



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2024 – 08:01 PM EST

PDB ID : 3PBP
Title : Structure of the yeast heterotrimeric Nup82-Nup159-Nup116 nucleoporin complex
Authors : Debler, E.W.; Hoelz, A.
Deposited on : 2010-10-20
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

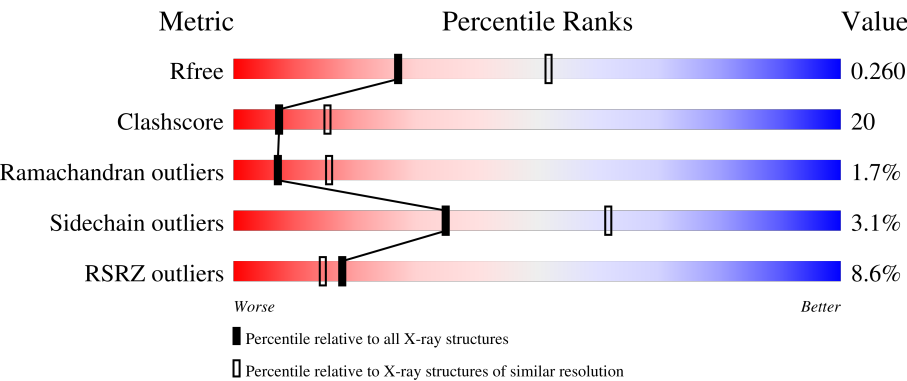
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	452	
1	D	452	
1	G	452	
1	J	452	
2	B	148	

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Mol	Chain	Length	Quality of chain
2	E	148	<div><div></div><div>20%59%35%5%•</div></div>
2	H	148	<div><div></div><div>30%54%42%••</div></div>
2	K	148	<div><div></div><div>14%57%39%••</div></div>
3	C	36	<div><div></div><div>3%39%31%•28%</div></div>
3	F	36	<div><div></div><div>8%44%25%•28%</div></div>
3	I	36	<div><div></div><div>3%56%19%•22%</div></div>
3	L	36	<div><div></div><div>3%50%17%33%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19653 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nucleoporin NUP82.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	Se	0	0	0
			3539	2273	569	686	4	7			
1	D	437	Total	C	N	O	S	Se	0	0	0
			3533	2270	568	684	4	7			
1	G	438	Total	C	N	O	S	Se	0	0	0
			3539	2273	569	686	4	7			
1	J	439	Total	C	N	O	S	Se	0	0	0
			3550	2279	573	687	4	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	SER	CYS	engineered mutation	UNP P40368
D	396	SER	CYS	engineered mutation	UNP P40368
G	396	SER	CYS	engineered mutation	UNP P40368
J	396	SER	CYS	engineered mutation	UNP P40368

- Molecule 2 is a protein called Nucleoporin NUP116/NSP116.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	Se	0	0	0
			1165	745	204	212	3	1			
2	E	146	Total	C	N	O	S	Se	0	0	0
			1165	745	204	212	3	1			
2	H	146	Total	C	N	O	S	Se	0	0	0
			1165	745	204	212	3	1			
2	K	146	Total	C	N	O	S	Se	0	0	0
			1165	745	204	212	3	1			

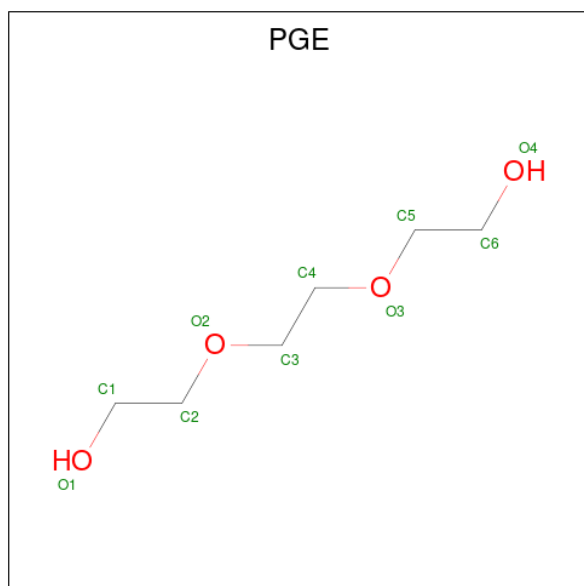
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	966	MSE	-	initiating methionine	UNP Q02630
E	966	MSE	-	initiating methionine	UNP Q02630
H	966	MSE	-	expression tag	UNP Q02630
K	966	MSE	-	initiating methionine	UNP Q02630

- Molecule 3 is a protein called Nucleoporin NUP159.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O	Se	0	0	0
			204	133	34	35	2			
3	F	26	Total	C	N	O	Se	0	0	0
			204	133	34	35	2			
3	I	28	Total	C	N	O	Se	0	0	0
			222	145	37	38	2			
3	L	24	Total	C	N	O	Se	0	0	0
			192	126	32	33	1			

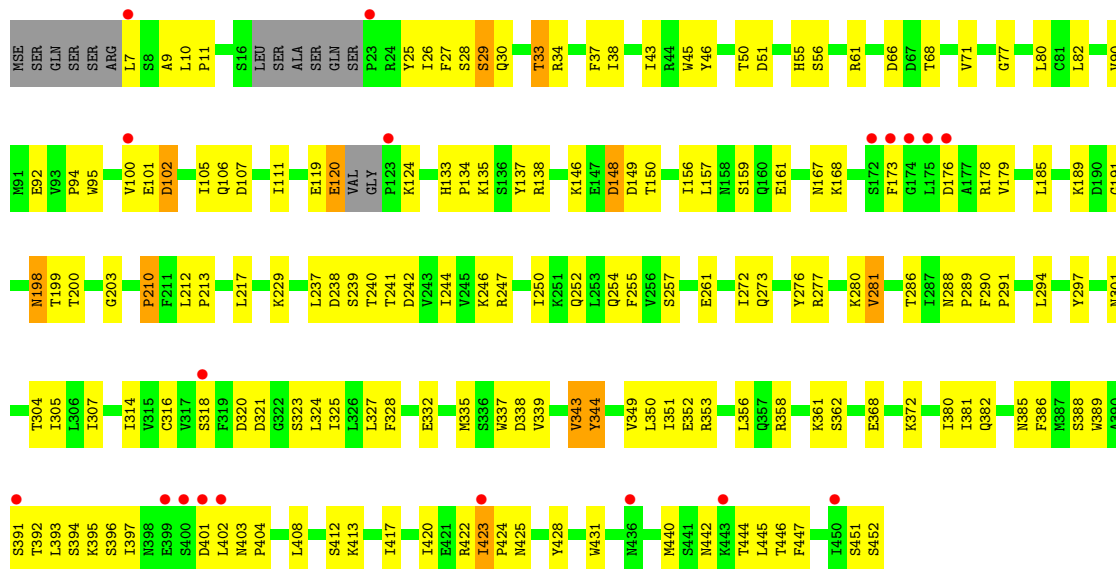
- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



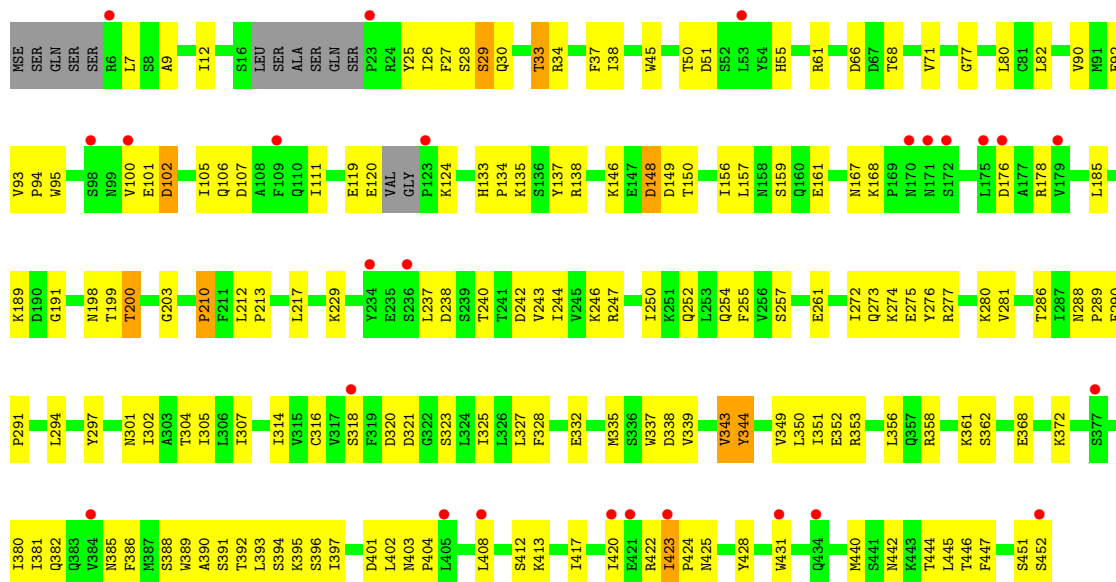
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			10	6	4		



• Molecule 1: Nucleoporin NUP82

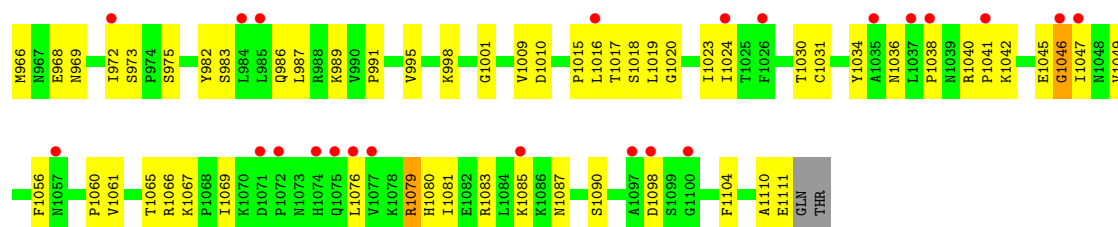


• Molecule 1: Nucleoporin NUP82

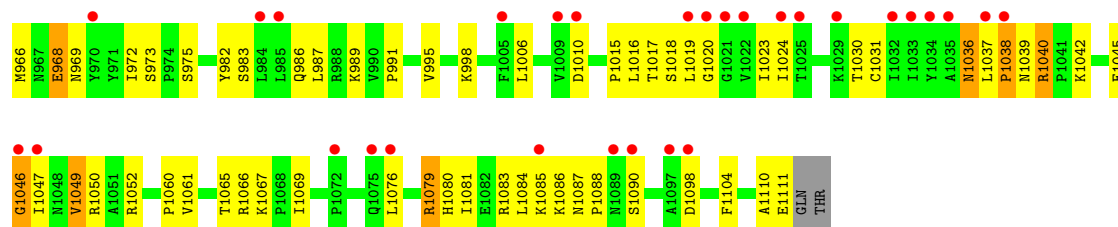


• Molecule 2: Nucleoporin NUP116/NSP116

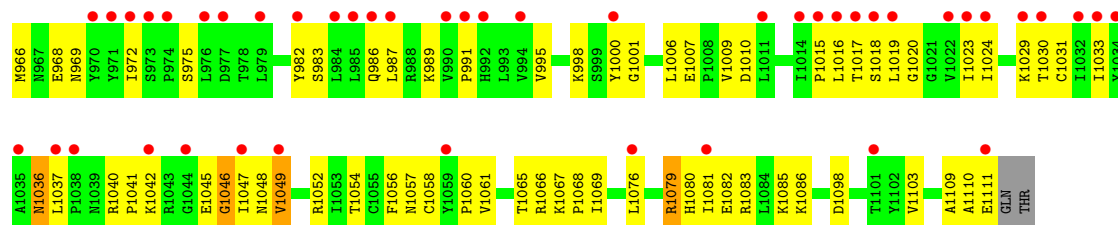




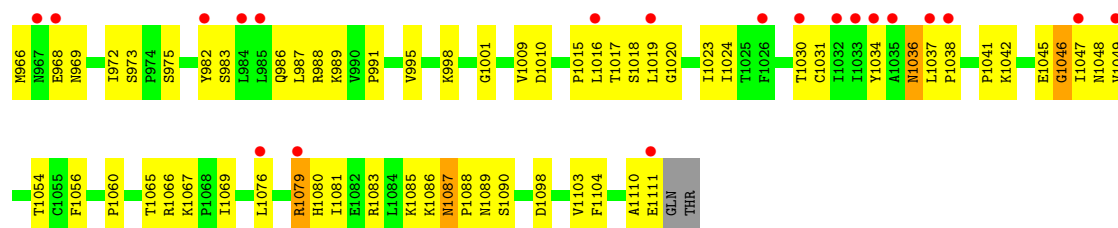
• Molecule 2: Nucleoporin NUP116/NSP116



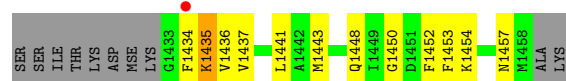
• Molecule 2: Nucleoporin NUP116/NSP116



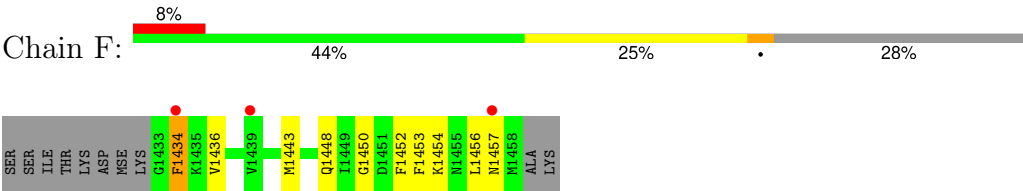
• Molecule 2: Nucleoporin NUP116/NSP116



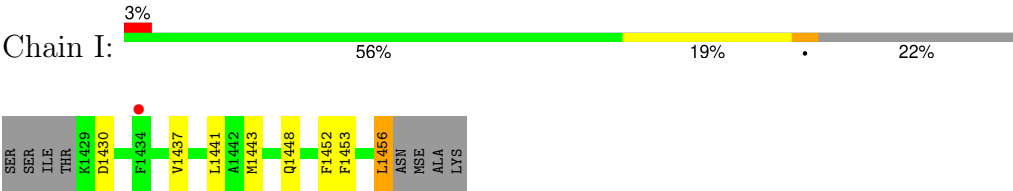
• Molecule 3: Nucleoporin NUP159



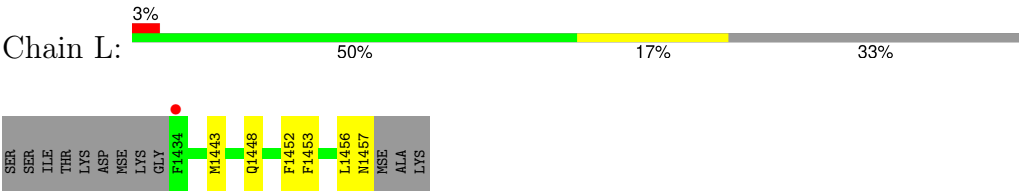
• Molecule 3: Nucleoporin NUP159



• Molecule 3: Nucleoporin NUP159



• Molecule 3: Nucleoporin NUP159



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.50Å 96.77Å 144.28Å 105.98° 93.97° 108.24°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.60) 93.3 (50.00-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.257 , 0.272 0.233 , 0.260	Depositor DCC
R_{free} test set	6890 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.889	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19653	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/3603	0.68	2/4877 (0.0%)
1	D	0.42	0/3597	0.68	2/4869 (0.0%)
1	G	0.42	0/3603	0.68	1/4877 (0.0%)
1	J	0.43	0/3614	0.68	1/4891 (0.0%)
2	B	0.35	0/1193	0.64	0/1617
2	E	0.35	0/1193	0.62	0/1617
2	H	0.41	0/1193	0.63	0/1617
2	K	0.37	0/1193	0.63	0/1617
3	C	0.53	0/204	0.61	0/266
3	F	0.48	0/204	0.56	0/266
3	I	0.44	0/222	0.64	0/288
3	L	0.49	0/193	0.52	0/254
All	All	0.41	0/20012	0.66	6/27056 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	343	VAL	N-CA-C	-5.42	96.38	111.00
1	G	343	VAL	N-CA-C	-5.15	97.09	111.00
1	D	343	VAL	N-CA-C	-5.10	97.23	111.00
1	A	343	VAL	N-CA-C	-5.05	97.36	111.00
1	A	381	ILE	N-CA-C	-5.04	97.38	111.00
1	D	381	ILE	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3539	0	3507	141	0
1	D	3533	0	3502	146	0
1	G	3539	0	3507	154	0
1	J	3550	0	3520	157	0
2	B	1165	0	1183	39	0
2	E	1165	0	1183	46	0
2	H	1165	0	1183	54	0
2	K	1165	0	1183	46	0
3	C	204	0	213	11	0
3	F	204	0	213	12	0
3	I	222	0	237	13	0
3	L	192	0	201	10	0
4	D	10	0	14	5	0
All	All	19653	0	19646	784	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (784) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1010:ASP:HB3	2:H:1046:GLY:HA2	1.41	0.99
1:G:10:LEU:HD12	1:G:11:PRO:HD2	1.51	0.92
1:J:444:THR:HG22	1:J:445:LEU:H	1.40	0.86
3:I:1437:VAL:HG11	1:J:243:VAL:HG12	1.58	0.85
1:G:444:THR:HG22	1:G:445:LEU:H	1.40	0.84
1:A:210:PRO:HG3	1:A:335:MSE:HE3	1.60	0.83
1:G:210:PRO:HG3	1:G:335:MSE:HE3	1.59	0.82
1:D:92:GLU:HB2	1:D:111:ILE:HD11	1.62	0.82
1:A:10:LEU:HD12	1:A:11:PRO:HD2	1.59	0.82
1:D:444:THR:HG22	1:D:445:LEU:H	1.41	0.81
1:J:90:VAL:HG11	1:J:156:ILE:HD13	1.62	0.81
1:A:210:PRO:CG	1:A:335:MSE:HE3	2.10	0.81
2:B:983:SER:HB2	2:B:986:GLN:HG2	1.63	0.81
2:E:983:SER:HB2	2:E:986:GLN:HG2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:PRO:CG	1:G:335:MSE:HE3	2.12	0.80
2:H:983:SER:HB2	2:H:986:GLN:HG2	1.64	0.80
1:G:90:VAL:HG11	1:G:156:ILE:HD13	1.62	0.80
1:A:92:GLU:HB2	1:A:111:ILE:HD11	1.64	0.79
1:D:148:ASP:HB3	1:D:150:THR:HB	1.64	0.79
1:A:444:THR:HG22	1:A:445:LEU:H	1.43	0.79
1:J:381:ILE:HD11	1:J:424:PRO:HG3	1.65	0.79
2:H:1001:GLY:HA2	2:H:1056:PHE:CE2	2.17	0.79
1:A:148:ASP:HB3	1:A:150:THR:HB	1.64	0.78
1:D:343:VAL:HG11	2:E:1066:ARG:NH1	1.98	0.78
1:A:90:VAL:HG11	1:A:156:ILE:HD13	1.65	0.78
1:D:90:VAL:HG11	1:D:156:ILE:HD13	1.64	0.78
1:D:210:PRO:CG	1:D:335:MSE:HE3	2.13	0.78
1:D:210:PRO:HG3	1:D:335:MSE:HE3	1.65	0.77
1:J:343:VAL:HG11	2:K:1066:ARG:NH1	1.99	0.77
1:J:210:PRO:HG3	1:J:335:MSE:HE3	1.66	0.77
2:K:983:SER:HB2	2:K:986:GLN:HG2	1.65	0.77
2:H:972:ILE:HD11	2:H:1019:LEU:HB2	1.67	0.77
1:D:381:ILE:HD11	1:D:424:PRO:HG3	1.66	0.77
2:E:1038:PRO:C	2:E:1040:ARG:H	1.85	0.77
1:J:210:PRO:CG	1:J:335:MSE:HE3	2.15	0.77
1:J:92:GLU:HB2	1:J:111:ILE:HD11	1.65	0.76
1:G:148:ASP:HB3	1:G:150:THR:HB	1.66	0.76
1:G:381:ILE:HD11	1:G:424:PRO:HG3	1.67	0.76
1:A:280:LYS:HD2	1:A:338:ASP:O	1.85	0.76
3:I:1441:LEU:HD11	1:J:243:VAL:HG13	1.68	0.76
1:D:358:ARG:CZ	1:D:380:ILE:HD12	2.17	0.75
1:J:148:ASP:HB3	1:J:150:THR:HB	1.67	0.75
1:J:358:ARG:CZ	1:J:380:ILE:HD12	2.16	0.75
1:J:392:THR:HG21	1:J:408:LEU:HD11	1.67	0.75
1:G:358:ARG:CZ	1:G:380:ILE:HD12	2.16	0.74
2:B:972:ILE:HD11	2:B:1019:LEU:HB2	1.69	0.74
1:G:92:GLU:HB2	1:G:111:ILE:HD11	1.67	0.74
1:G:255:PHE:CD2	1:G:335:MSE:HE1	2.22	0.74
1:G:280:LYS:HD2	1:G:338:ASP:O	1.87	0.74
1:J:361:LYS:HE2	1:J:423:ILE:HD11	1.69	0.74
1:D:289:PRO:HG3	3:F:1457:ASN:HB2	1.69	0.74
1:G:119:GLU:O	1:G:124:LYS:HE2	1.88	0.74
1:D:27:PHE:HZ	1:D:71:VAL:HG23	1.53	0.73
1:J:119:GLU:O	1:J:124:LYS:HE2	1.88	0.73
1:A:358:ARG:CZ	1:A:380:ILE:HD12	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ILE:HD11	1:A:424:PRO:HG3	1.68	0.73
1:D:189:LYS:HG2	1:D:304:THR:CG2	2.19	0.73
1:D:392:THR:HG21	1:D:408:LEU:HD11	1.70	0.73
1:A:361:LYS:HE2	1:A:423:ILE:HD11	1.70	0.73
1:D:280:LYS:HD2	1:D:338:ASP:O	1.87	0.73
1:J:343:VAL:HG11	2:K:1066:ARG:CZ	2.19	0.73
1:D:66:ASP:OD1	1:D:68:THR:HB	1.88	0.73
1:A:392:THR:HG21	1:A:408:LEU:HD11	1.72	0.72
1:J:66:ASP:OD1	1:J:68:THR:HB	1.89	0.72
1:J:335:MSE:HE2	1:J:337:TRP:CZ2	2.25	0.72
2:K:1086:LYS:O	2:K:1087:ASN:HB3	1.88	0.72
2:K:972:ILE:HD11	2:K:1019:LEU:HB2	1.69	0.72
1:A:66:ASP:OD1	1:A:68:THR:HB	1.89	0.72
1:G:66:ASP:OD1	1:G:68:THR:HB	1.90	0.72
1:G:189:LYS:HG2	1:G:304:THR:CG2	2.19	0.72
1:J:37:PHE:HE1	1:J:440:MSE:HE1	1.54	0.72
1:D:335:MSE:HE2	1:D:337:TRP:CZ2	2.23	0.72
1:D:444:THR:HG22	1:D:445:LEU:N	2.04	0.72
1:A:119:GLU:O	1:A:124:LYS:HE2	1.89	0.72
1:A:335:MSE:HE2	1:A:337:TRP:CZ2	2.24	0.72
1:J:255:PHE:CD2	1:J:335:MSE:HE1	2.25	0.72
1:J:444:THR:HG22	1:J:445:LEU:N	2.05	0.72
2:E:972:ILE:HD11	2:E:1019:LEU:HB2	1.70	0.71
1:G:392:THR:HG21	1:G:408:LEU:HD11	1.72	0.71
1:G:361:LYS:HE2	1:G:423:ILE:HD11	1.72	0.71
1:G:444:THR:HG22	1:G:445:LEU:N	2.05	0.71
1:D:119:GLU:O	1:D:124:LYS:HE2	1.90	0.71
1:J:280:LYS:HD2	1:J:338:ASP:O	1.89	0.71
2:K:1090:SER:HB2	2:K:1104:PHE:CD2	2.25	0.71
1:A:27:PHE:HZ	1:A:71:VAL:HG23	1.55	0.70
3:C:1434:PHE:O	3:C:1436:VAL:N	2.24	0.70
1:J:27:PHE:HZ	1:J:71:VAL:HG23	1.54	0.70
1:J:237:LEU:HD22	1:J:246:LYS:HG3	1.73	0.70
1:G:27:PHE:HZ	1:G:71:VAL:HG23	1.55	0.70
1:G:173:PHE:HE2	2:H:1033:ILE:HD12	1.56	0.70
1:A:444:THR:HG22	1:A:445:LEU:N	2.06	0.70
1:D:255:PHE:CD2	1:D:335:MSE:HE1	2.26	0.70
1:G:335:MSE:HE2	1:G:337:TRP:CZ2	2.27	0.69
1:A:189:LYS:HG2	1:A:304:THR:CG2	2.22	0.69
1:G:7:LEU:HB2	1:G:431:TRP:CZ3	2.27	0.69
1:A:255:PHE:CD2	1:A:335:MSE:HE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ARG:HB3	1:D:95:TRP:CH2	2.28	0.69
1:D:361:LYS:HE2	1:D:423:ILE:HD11	1.74	0.69
1:D:440:MSE:HE2	1:D:445:LEU:HD13	1.75	0.69
2:K:1010:ASP:HB3	2:K:1046:GLY:HA2	1.75	0.69
2:H:989:LYS:O	2:H:991:PRO:HD3	1.94	0.68
1:J:325:ILE:HD12	1:J:327:LEU:HD21	1.75	0.68
2:E:989:LYS:O	2:E:991:PRO:HD3	1.94	0.67
2:H:1042:LYS:O	2:H:1045:GLU:HB2	1.95	0.67
1:G:343:VAL:HG11	2:H:1066:ARG:NH1	2.10	0.67
2:K:989:LYS:O	2:K:991:PRO:HD3	1.94	0.67
2:B:989:LYS:O	2:B:991:PRO:HD3	1.95	0.66
2:K:1037:LEU:N	2:K:1038:PRO:HD3	2.09	0.66
2:B:1042:LYS:O	2:B:1045:GLU:HB2	1.95	0.66
1:A:15:ALA:HB2	1:A:24:ARG:HH21	1.61	0.66
1:D:301:ASN:H	1:D:318:SER:HB2	1.61	0.66
1:J:422:ARG:HG3	1:J:442:ASN:HD21	1.58	0.66
3:I:1437:VAL:CG1	1:J:243:VAL:HG12	2.25	0.66
1:A:325:ILE:HD12	1:A:327:LEU:HD21	1.78	0.66
1:A:440:MSE:HE2	1:A:445:LEU:HD13	1.78	0.66
1:J:335:MSE:HE2	1:J:337:TRP:CH2	2.31	0.65
1:A:422:ARG:HG3	1:A:442:ASN:HD21	1.61	0.65
1:D:422:ARG:HG3	1:D:442:ASN:HD21	1.61	0.65
2:H:1010:ASP:HB3	2:H:1046:GLY:CA	2.21	0.65
1:J:189:LYS:HG2	1:J:304:THR:CG2	2.26	0.65
1:J:440:MSE:HE2	1:J:445:LEU:HD13	1.76	0.65
1:D:343:VAL:HG11	2:E:1066:ARG:CZ	2.26	0.65
1:G:440:MSE:HE2	1:G:445:LEU:HD13	1.78	0.65
1:D:30:GLN:O	1:D:33:THR:HB	1.97	0.65
2:H:1082:GLU:HG2	2:H:1086:LYS:HE3	1.79	0.65
1:J:30:GLN:O	1:J:33:THR:HB	1.96	0.65
1:A:92:GLU:HB2	1:A:111:ILE:CD1	2.26	0.64
1:J:34:ARG:HB3	1:J:95:TRP:CH2	2.31	0.64
1:J:92:GLU:HB2	1:J:111:ILE:CD1	2.26	0.64
1:G:34:ARG:HB3	1:G:95:TRP:CH2	2.32	0.64
1:G:255:PHE:CE2	1:G:335:MSE:HE1	2.32	0.64
1:A:301:ASN:H	1:A:318:SER:HB2	1.63	0.64
1:G:335:MSE:HE2	1:G:337:TRP:CH2	2.32	0.64
1:G:422:ARG:HG3	1:G:442:ASN:HD21	1.61	0.64
1:J:307:ILE:HD11	1:J:314:ILE:HD11	1.78	0.64
2:B:1090:SER:HB2	2:B:1104:PHE:CD2	2.33	0.64
1:G:30:GLN:O	1:G:33:THR:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1042:LYS:O	2:K:1045:GLU:HB2	1.97	0.64
2:K:1069:ILE:HD12	2:K:1076:LEU:HD12	1.80	0.64
1:A:30:GLN:O	1:A:33:THR:HB	1.98	0.64
1:A:34:ARG:HB3	1:A:95:TRP:CH2	2.33	0.64
2:E:1042:LYS:O	2:E:1045:GLU:HB2	1.97	0.64
1:D:25:TYR:CD2	1:D:71:VAL:HG22	2.33	0.63
1:D:92:GLU:HB2	1:D:111:ILE:CD1	2.26	0.63
1:G:25:TYR:CD2	1:G:71:VAL:HG22	2.34	0.63
1:J:255:PHE:CE2	1:J:335:MSE:HE1	2.34	0.63
1:G:92:GLU:HB2	1:G:111:ILE:CD1	2.28	0.63
1:J:301:ASN:H	1:J:318:SER:HB2	1.64	0.63
1:G:29:SER:OG	1:G:77:GLY:HA3	1.98	0.63
1:A:335:MSE:HE2	1:A:337:TRP:CH2	2.34	0.62
1:D:335:MSE:HE2	1:D:337:TRP:CH2	2.33	0.62
1:G:301:ASN:H	1:G:318:SER:HB2	1.63	0.62
2:B:1015:PRO:HG2	2:B:1018:SER:OG	1.99	0.62
1:D:26:ILE:HB	1:D:440:MSE:HE3	1.80	0.62
1:D:255:PHE:CE2	1:D:335:MSE:HE1	2.34	0.62
1:G:380:ILE:HG22	1:G:381:ILE:N	2.14	0.62
1:J:37:PHE:HE1	1:J:440:MSE:CE	2.12	0.62
1:J:402:LEU:HD21	3:L:1448:GLN:HB3	1.79	0.62
1:G:100:VAL:HG12	1:G:106:GLN:HG2	1.82	0.62
2:E:1069:ILE:HD12	2:E:1076:LEU:HD12	1.82	0.62
1:G:307:ILE:HD11	1:G:314:ILE:HD11	1.80	0.62
1:A:25:TYR:CD2	1:A:71:VAL:HG22	2.34	0.62
1:J:444:THR:CG2	1:J:445:LEU:H	2.13	0.62
2:E:1015:PRO:HG2	2:E:1018:SER:OG	2.00	0.62
2:H:1015:PRO:HG2	2:H:1018:SER:OG	2.00	0.62
1:A:372:LYS:HE2	1:A:385:ASN:ND2	2.16	0.61
1:A:255:PHE:CE2	1:A:335:MSE:HE1	2.35	0.61
1:D:100:VAL:HG12	1:D:106:GLN:HG2	1.80	0.61
1:D:380:ILE:HG22	1:D:381:ILE:N	2.14	0.61
1:A:38:ILE:HD11	1:A:80:LEU:HD13	1.83	0.61
1:A:146:LYS:HB2	1:A:150:THR:HG22	1.82	0.61
2:B:1069:ILE:HD12	2:B:1076:LEU:HD12	1.82	0.61
1:D:148:ASP:O	1:D:149:ASP:HB2	2.00	0.61
2:H:1069:ILE:HD12	2:H:1076:LEU:HD12	1.81	0.61
1:A:148:ASP:O	1:A:149:ASP:HB2	2.00	0.61
2:K:1015:PRO:HG2	2:K:1018:SER:OG	1.99	0.61
1:D:372:LYS:HE2	1:D:385:ASN:ND2	2.16	0.61
1:J:380:ILE:HG22	1:J:381:ILE:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ILE:HG22	1:A:381:ILE:N	2.14	0.61
1:D:146:LYS:HB2	1:D:150:THR:HG22	1.81	0.61
1:D:297:TYR:HB3	1:D:320:ASP:HB2	1.83	0.61
1:J:100:VAL:HG12	1:J:106:GLN:HG2	1.83	0.61
2:B:1040:ARG:N	2:B:1041:PRO:HD3	2.15	0.61
1:D:307:ILE:HD11	1:D:314:ILE:HD11	1.83	0.61
1:G:148:ASP:O	1:G:149:ASP:HB2	2.00	0.61
1:A:343:VAL:O	1:A:344:TYR:HB2	2.01	0.60
1:D:38:ILE:HD11	1:D:80:LEU:HD13	1.84	0.60
1:A:307:ILE:HD11	1:A:314:ILE:HD11	1.84	0.60
1:G:444:THR:CG2	1:G:445:LEU:H	2.13	0.60
2:K:1081:ILE:HG22	2:K:1085:LYS:HE3	1.84	0.60
1:J:148:ASP:O	1:J:149:ASP:HB2	2.02	0.60
1:J:25:TYR:CD2	1:J:71:VAL:HG22	2.37	0.60
1:A:297:TYR:HB3	1:A:320:ASP:HB2	1.84	0.60
1:G:38:ILE:HD11	1:G:80:LEU:HD13	1.84	0.60
1:G:146:LYS:HB2	1:G:150:THR:HG22	1.84	0.59
1:J:372:LYS:HE2	1:J:385:ASN:ND2	2.16	0.59
2:K:1065:THR:HG22	2:K:1067:LYS:HG3	1.83	0.59
1:D:325:ILE:HD12	1:D:327:LEU:HD21	1.84	0.59
1:G:325:ILE:HD12	1:G:327:LEU:HD21	1.84	0.59
1:G:10:LEU:HD21	1:G:46:TYR:CE2	2.37	0.59
1:G:343:VAL:O	1:G:344:TYR:HB2	2.03	0.59
1:J:82:LEU:HD12	1:J:82:LEU:N	2.17	0.59
1:A:100:VAL:HG12	1:A:106:GLN:HG2	1.83	0.59
1:D:343:VAL:O	1:D:344:TYR:HB2	2.02	0.59
2:H:1110:ALA:O	2:H:1111:GLU:HG3	2.03	0.59
2:K:969:ASN:O	2:K:998:LYS:HG3	2.03	0.59
1:G:37:PHE:HE1	1:G:440:MSE:HE1	1.68	0.58
1:J:297:TYR:HB3	1:J:320:ASP:HB2	1.84	0.58
2:H:1081:ILE:HG22	2:H:1085:LYS:HE3	1.85	0.58
1:A:343:VAL:HG11	2:B:1066:ARG:NH1	2.18	0.58
2:H:1029:LYS:HE2	2:H:1057:ASN:O	2.03	0.58
1:G:372:LYS:HE2	1:G:385:ASN:ND2	2.17	0.58
1:A:289:PRO:HG3	3:C:1457:ASN:HB2	1.85	0.58
1:J:386:PHE:HB3	1:J:412:SER:OG	2.03	0.58
2:B:1110:ALA:O	2:B:1111:GLU:HG3	2.04	0.58
1:A:305:ILE:HD12	1:A:305:ILE:N	2.19	0.58
1:D:349:VAL:HG11	3:F:1453:PHE:HB2	1.85	0.58
1:G:386:PHE:HB3	1:G:412:SER:OG	2.04	0.58
2:E:1065:THR:HG22	2:E:1067:LYS:HG3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:ILE:HB	1:G:440:MSE:HE3	1.86	0.57
1:D:402:LEU:HD21	3:F:1448:GLN:HB3	1.84	0.57
1:D:444:THR:CG2	1:D:445:LEU:H	2.14	0.57
1:G:305:ILE:N	1:G:305:ILE:HD12	2.19	0.57
3:I:1437:VAL:CG1	1:J:243:VAL:CG1	2.82	0.57
1:G:297:TYR:HB3	1:G:320:ASP:HB2	1.85	0.57
3:L:1452:PHE:CE1	3:L:1456:LEU:HD22	2.39	0.57
1:G:349:VAL:HG11	3:I:1453:PHE:HB2	1.86	0.57
1:A:444:THR:CG2	1:A:445:LEU:H	2.15	0.57
2:B:966:MSE:HG3	2:B:1020:GLY:HA3	1.86	0.57
1:J:307:ILE:HD11	1:J:314:ILE:CD1	2.34	0.57
1:J:343:VAL:O	1:J:344:TYR:HB2	2.05	0.57
2:K:1110:ALA:O	2:K:1111:GLU:HG3	2.04	0.57
1:A:257:SER:O	1:A:261:GLU:HG3	2.04	0.57
2:B:1065:THR:HG22	2:B:1067:LYS:HG3	1.85	0.57
2:B:1081:ILE:HG22	2:B:1085:LYS:HE3	1.85	0.57
1:D:29:SER:OG	1:D:77:GLY:HA3	2.05	0.57
1:G:257:SER:O	1:G:261:GLU:HG3	2.05	0.57
2:B:983:SER:CB	2:B:986:GLN:HG2	2.35	0.56
2:H:1065:THR:HG22	2:H:1067:LYS:HG3	1.87	0.56
3:I:1456:LEU:HD12	3:I:1456:LEU:O	2.05	0.56
1:J:146:LYS:HB2	1:J:150:THR:HG22	1.87	0.56
1:J:440:MSE:CE	1:J:445:LEU:HD13	2.35	0.56
1:A:29:SER:OG	1:A:77:GLY:HA3	2.05	0.56
1:A:29:SER:HB3	1:A:34:ARG:HD3	1.87	0.56
3:C:1434:PHE:C	3:C:1436:VAL:H	2.08	0.56
2:E:983:SER:CB	2:E:986:GLN:HG2	2.35	0.56
2:H:966:MSE:HG3	2:H:1020:GLY:HA3	1.87	0.56
1:J:305:ILE:N	1:J:305:ILE:HD12	2.21	0.56
2:K:966:MSE:HG3	2:K:1020:GLY:HA3	1.86	0.56
2:K:1065:THR:HG21	2:K:1067:LYS:HD2	1.88	0.56
2:E:1065:THR:HG21	2:E:1067:LYS:HD2	1.86	0.56
2:H:1010:ASP:CB	2:H:1046:GLY:HA2	2.27	0.56
2:E:1081:ILE:HG22	2:E:1085:LYS:HE3	1.86	0.56
1:G:82:LEU:HD12	1:G:82:LEU:N	2.21	0.56
1:D:276:TYR:CE2	4:D:6119:PGE:H5	2.40	0.56
2:H:969:ASN:O	2:H:998:LYS:HG3	2.06	0.56
1:D:257:SER:O	1:D:261:GLU:HG3	2.05	0.56
1:J:242:ASP:OD1	1:J:244:ILE:N	2.39	0.56
2:E:1110:ALA:O	2:E:1111:GLU:HG3	2.06	0.56
1:J:38:ILE:HD11	1:J:80:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:SER:HB3	1:G:34:ARG:HD3	1.87	0.56
1:A:402:LEU:HD21	3:C:1448:GLN:HB3	1.88	0.55
1:D:242:ASP:OD1	1:D:244:ILE:N	2.39	0.55
1:J:29:SER:HB3	1:J:34:ARG:HD3	1.87	0.55
2:B:1010:ASP:HB3	2:B:1046:GLY:HA2	1.87	0.55
3:F:1434:PHE:CD1	3:F:1434:PHE:N	2.73	0.55
1:J:29:SER:OG	1:J:77:GLY:HA3	2.06	0.55
2:B:1065:THR:HG21	2:B:1067:LYS:HD2	1.87	0.55
2:B:969:ASN:O	2:B:998:LYS:HG3	2.06	0.55
2:E:969:ASN:O	2:E:998:LYS:HG3	2.05	0.55
2:H:983:SER:CB	2:H:986:GLN:HG2	2.35	0.55
1:A:386:PHE:HB3	1:A:412:SER:OG	2.06	0.55
2:K:1041:PRO:HB2	2:K:1048:ASN:HB2	1.88	0.55
2:H:1065:THR:HG21	2:H:1067:LYS:HD2	1.89	0.55
1:A:343:VAL:HG11	2:B:1066:ARG:CZ	2.37	0.55
1:J:257:SER:O	1:J:261:GLU:HG3	2.07	0.55
1:J:381:ILE:HD11	1:J:420:ILE:HG21	1.89	0.55
2:E:966:MSE:HG3	2:E:1020:GLY:HA3	1.88	0.54
1:D:386:PHE:HB3	1:D:412:SER:OG	2.07	0.54
1:G:10:LEU:CD1	1:G:11:PRO:HD2	2.31	0.54
2:H:995:VAL:HG21	2:H:1024:ILE:HD12	1.88	0.54
1:A:210:PRO:HG3	1:A:335:MSE:CE	2.34	0.54
1:G:37:PHE:HE1	1:G:440:MSE:CE	2.21	0.54
1:J:189:LYS:NZ	1:J:304:THR:HG22	2.21	0.54
1:D:137:TYR:CE2	1:D:138:ARG:HG3	2.43	0.54
1:J:332:GLU:CB	3:L:1443:MSE:HE3	2.38	0.54
1:G:307:ILE:HD11	1:G:314:ILE:CD1	2.38	0.54
1:D:202:GLY:HA2	2:E:1079:ARG:HH12	1.72	0.54
1:G:210:PRO:HG3	1:G:335:MSE:CE	2.37	0.53
2:K:1001:GLY:HA2	2:K:1056:PHE:CE2	2.43	0.53
1:G:402:LEU:HD21	3:I:1448:GLN:HB3	1.91	0.53
1:J:402:LEU:HD21	3:L:1448:GLN:CB	2.38	0.53
1:G:332:GLU:CB	3:I:1443:MSE:HE3	2.39	0.53
2:K:1017:THR:HG22	2:K:1017:THR:O	2.08	0.53
1:A:349:VAL:HG11	3:C:1453:PHE:HB2	1.90	0.53
1:D:212:LEU:O	1:D:277:ARG:HD2	2.08	0.53
1:G:10:LEU:HD21	1:G:46:TYR:HE2	1.73	0.53
1:A:26:ILE:HB	1:A:440:MSE:HE3	1.90	0.53
2:H:982:TYR:HB2	2:H:987:LEU:HD13	1.90	0.53
1:A:242:ASP:OD1	1:A:244:ILE:N	2.42	0.53
1:D:7:LEU:HB2	1:D:431:TRP:CZ3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:ASP:OD1	1:G:244:ILE:N	2.41	0.53
1:G:173:PHE:CZ	2:H:1109:ALA:O	2.62	0.53
1:A:82:LEU:N	1:A:82:LEU:HD12	2.24	0.53
1:A:138:ARG:NH2	1:A:157:LEU:HD13	2.24	0.53
1:A:380:ILE:CG2	1:A:381:ILE:N	2.71	0.53
1:G:199:THR:HG22	1:G:199:THR:O	2.09	0.53
1:D:307:ILE:HD11	1:D:314:ILE:CD1	2.39	0.52
2:H:1000:TYR:C	2:H:1056:PHE:CD2	2.83	0.52
2:K:982:TYR:HB2	2:K:987:LEU:HD13	1.91	0.52
2:K:1009:VAL:HG13	2:K:1046:GLY:O	2.10	0.52
1:D:82:LEU:N	1:D:82:LEU:HD12	2.24	0.52
1:D:402:LEU:HD21	3:F:1448:GLN:CB	2.40	0.52
1:J:381:ILE:HD11	1:J:424:PRO:CG	2.38	0.52
1:D:305:ILE:HD12	1:D:305:ILE:N	2.24	0.52
1:D:380:ILE:CG2	1:D:381:ILE:N	2.72	0.52
1:G:380:ILE:CG2	1:G:381:ILE:N	2.72	0.52
1:J:289:PRO:HG3	3:L:1457:ASN:HB2	1.92	0.52
1:D:27:PHE:CZ	1:D:71:VAL:HG23	2.40	0.52
2:E:1037:LEU:N	2:E:1038:PRO:HD3	2.24	0.52
1:D:29:SER:HB3	1:D:34:ARG:HD3	1.90	0.52
2:B:1017:THR:O	2:B:1017:THR:HG22	2.10	0.52
1:J:356:LEU:O	1:J:358:ARG:HG3	2.10	0.52
3:I:1441:LEU:CD1	1:J:243:VAL:HG13	2.38	0.52
2:K:995:VAL:HG21	2:K:1024:ILE:HD12	1.91	0.52
1:D:138:ARG:NH2	1:D:157:LEU:HD13	2.25	0.52
1:A:307:ILE:HD11	1:A:314:ILE:CD1	2.40	0.51
1:G:381:ILE:HD11	1:G:420:ILE:HG21	1.92	0.51
1:J:138:ARG:NH2	1:J:157:LEU:HD13	2.25	0.51
1:J:422:ARG:CG	1:J:442:ASN:HD21	2.22	0.51
2:K:1087:ASN:C	2:K:1089:ASN:H	2.13	0.51
1:A:440:MSE:CE	1:A:445:LEU:HD13	2.39	0.51
1:G:138:ARG:NH2	1:G:157:LEU:HD13	2.25	0.51
1:D:440:MSE:CE	1:D:445:LEU:HD13	2.39	0.51
2:E:995:VAL:HG21	2:E:1024:ILE:HD12	1.92	0.51
1:J:393:LEU:O	1:J:397:ILE:HG13	2.10	0.51
2:K:983:SER:CB	2:K:986:GLN:HG2	2.35	0.51
1:D:393:LEU:O	1:D:397:ILE:HG13	2.11	0.51
1:D:403:ASN:HB2	1:D:404:PRO:HD3	1.93	0.51
1:D:422:ARG:O	1:D:423:ILE:C	2.49	0.51
1:G:27:PHE:CZ	1:G:71:VAL:HG23	2.42	0.51
1:J:238:ASP:OD2	1:J:240:THR:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:321:ASP:OD2	1:J:323:SER:HB2	2.09	0.51
1:A:420:ILE:HG21	1:A:424:PRO:HG3	1.93	0.51
1:J:349:VAL:HG11	3:L:1453:PHE:HB2	1.92	0.51
1:J:403:ASN:HB2	1:J:404:PRO:HD3	1.92	0.51
1:G:422:ARG:O	1:G:423:ILE:C	2.49	0.51
1:J:380:ILE:CG2	1:J:381:ILE:N	2.73	0.51
1:A:381:ILE:HD11	1:A:420:ILE:HG21	1.93	0.51
1:D:332:GLU:CB	3:F:1443:MSE:HE3	2.41	0.51
1:A:210:PRO:CB	1:A:335:MSE:HE3	2.40	0.51
1:J:27:PHE:CZ	1:J:71:VAL:HG23	2.40	0.51
1:A:393:LEU:O	1:A:397:ILE:HG13	2.11	0.50
1:D:381:ILE:HD11	1:D:420:ILE:HG21	1.92	0.50
2:E:1017:THR:O	2:E:1017:THR:HG22	2.11	0.50
1:G:238:ASP:OD2	1:G:240:THR:N	2.40	0.50
1:A:199:THR:HG22	1:A:199:THR:O	2.10	0.50
1:G:356:LEU:O	1:G:358:ARG:HG3	2.12	0.50
1:J:199:THR:O	1:J:199:THR:HG22	2.10	0.50
1:A:237:LEU:HD22	1:A:246:LYS:HG3	1.93	0.50
1:D:210:PRO:HG3	1:D:335:MSE:CE	2.39	0.50
2:H:1009:VAL:HG13	2:H:1046:GLY:O	2.10	0.50
1:J:137:TYR:CE2	1:J:138:ARG:HG3	2.46	0.50
1:A:388:SER:OG	1:A:413:LYS:HE3	2.11	0.50
3:L:1456:LEU:HG	3:L:1456:LEU:O	2.11	0.50
1:G:388:SER:OG	1:G:413:LYS:HE3	2.12	0.50
1:G:420:ILE:HG21	1:G:424:PRO:HG3	1.94	0.50
1:A:37:PHE:HE1	1:A:440:MSE:CE	2.25	0.50
2:B:1001:GLY:HA2	2:B:1056:PHE:CE2	2.47	0.50
2:H:1017:THR:HG22	2:H:1017:THR:O	2.12	0.50
1:J:210:PRO:CB	1:J:335:MSE:HE3	2.42	0.50
1:J:425:ASN:HB3	1:J:440:MSE:HB3	1.94	0.50
1:A:250:ILE:O	1:A:254:GLN:HG3	2.11	0.50
1:A:422:ARG:O	1:A:423:ILE:C	2.50	0.50
1:D:237:LEU:HD22	1:D:246:LYS:HG3	1.93	0.50
1:G:250:ILE:O	1:G:254:GLN:HG3	2.12	0.50
1:G:381:ILE:HD11	1:G:424:PRO:CG	2.38	0.50
1:A:403:ASN:HB2	1:A:404:PRO:HD3	1.94	0.50
1:G:7:LEU:HB2	1:G:431:TRP:CH2	2.46	0.50
1:A:446:THR:HG22	1:A:447:PHE:N	2.26	0.49
1:J:325:ILE:HG13	1:J:325:ILE:O	2.12	0.49
1:G:167:ASN:O	1:G:178:ARG:NH1	2.43	0.49
1:A:356:LEU:O	1:A:358:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:THR:HG22	1:D:34:ARG:HG3	1.94	0.49
1:G:403:ASN:HB2	1:G:404:PRO:HD3	1.93	0.49
1:J:422:ARG:O	1:J:423:ILE:C	2.50	0.49
1:A:27:PHE:CZ	1:A:71:VAL:HG23	2.42	0.49
2:B:995:VAL:HG21	2:B:1024:ILE:HD12	1.93	0.49
1:G:440:MSE:CE	1:G:445:LEU:HD13	2.40	0.49
1:A:343:VAL:O	1:A:344:TYR:CB	2.61	0.49
1:D:199:THR:HG22	1:D:199:THR:O	2.12	0.49
1:G:45:TRP:CZ2	1:G:94:PRO:HB2	2.47	0.49
1:A:332:GLU:CB	3:C:1443:MSE:HE3	2.43	0.49
1:A:425:ASN:HB3	1:A:440:MSE:HB3	1.94	0.49
1:D:189:LYS:HG2	1:D:304:THR:HG21	1.91	0.49
1:D:212:LEU:HD13	1:D:272:ILE:HD13	1.95	0.49
1:D:356:LEU:O	1:D:358:ARG:HG3	2.13	0.49
2:E:1018:SER:HB3	2:E:1023:ILE:HG13	1.94	0.49
1:G:30:GLN:CG	1:G:34:ARG:HD2	2.42	0.49
1:G:240:THR:HG22	1:G:240:THR:O	2.12	0.49
1:G:425:ASN:HB3	1:G:440:MSE:HB3	1.94	0.49
1:D:250:ILE:O	1:D:254:GLN:HG3	2.12	0.49
1:G:189:LYS:HG2	1:G:304:THR:HG22	1.94	0.49
2:E:982:TYR:HB2	2:E:987:LEU:HD13	1.93	0.49
1:A:167:ASN:O	1:A:178:ARG:NH1	2.46	0.48
1:A:392:THR:CG2	1:A:408:LEU:HD11	2.43	0.48
2:B:982:TYR:HB2	2:B:987:LEU:HD13	1.93	0.48
1:D:45:TRP:CZ2	1:D:94:PRO:HB2	2.48	0.48
1:J:392:THR:CG2	1:J:408:LEU:HD11	2.41	0.48
1:A:444:THR:CG2	1:A:445:LEU:N	2.75	0.48
1:D:45:TRP:CE2	1:D:55:HIS:HB2	2.49	0.48
1:D:210:PRO:CB	1:D:335:MSE:HE3	2.43	0.48
1:J:30:GLN:CG	1:J:34:ARG:HD2	2.44	0.48
1:A:45:TRP:CZ2	1:A:94:PRO:HB2	2.48	0.48
1:A:189:LYS:HG2	1:A:304:THR:HG22	1.95	0.48
1:A:381:ILE:HD11	1:A:424:PRO:CG	2.39	0.48
1:D:189:LYS:HG2	1:D:304:THR:HG22	1.95	0.48
1:D:343:VAL:O	1:D:344:TYR:CB	2.62	0.48
1:D:422:ARG:CG	1:D:442:ASN:HD21	2.25	0.48
3:L:1453:PHE:O	3:L:1457:ASN:ND2	2.43	0.48
1:D:133:HIS:CE1	1:D:213:PRO:HD3	2.49	0.48
1:G:273:GLN:OE1	1:G:276:TYR:HE1	1.97	0.48
1:G:325:ILE:O	1:G:325:ILE:HG13	2.14	0.48
1:G:451:SER:O	1:G:452:SER:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:420:ILE:HG21	1:J:424:PRO:HG3	1.95	0.48
1:J:451:SER:O	1:J:452:SER:HB3	2.13	0.48
1:A:61:ARG:NH1	1:A:107:ASP:OD1	2.46	0.48
3:F:1456:LEU:O	3:F:1456:LEU:HG	2.14	0.48
1:J:391:SER:O	1:J:395:LYS:HG3	2.14	0.48
1:D:420:ILE:HG21	1:D:424:PRO:HG3	1.96	0.48
1:D:446:THR:HG22	1:D:447:PHE:N	2.28	0.48
1:D:9:ALA:O	1:D:10:LEU:C	2.52	0.48
1:A:198:ASN:O	1:A:203:GLY:HA2	2.14	0.48
1:A:422:ARG:CG	1:A:442:ASN:HD21	2.26	0.48
1:D:381:ILE:HD11	1:D:424:PRO:CG	2.38	0.48
1:D:425:ASN:HB3	1:D:440:MSE:HB3	1.95	0.48
1:D:451:SER:O	1:D:452:SER:HB3	2.13	0.48
2:E:1038:PRO:C	2:E:1040:ARG:N	2.57	0.48
3:F:1452:PHE:CE1	3:F:1456:LEU:HD22	2.49	0.48
1:G:237:LEU:HD22	1:G:246:LYS:HG3	1.96	0.48
1:J:250:ILE:O	1:J:254:GLN:HG3	2.14	0.48
1:A:321:ASP:OD2	1:A:323:SER:HB2	2.14	0.48
1:J:229:LYS:HE3	1:J:332:GLU:CD	2.34	0.48
1:J:189:LYS:HZ3	1:J:304:THR:HG22	1.79	0.47
2:B:1018:SER:HB3	2:B:1023:ILE:HG13	1.96	0.47
2:H:1036:ASN:O	2:H:1037:LEU:HB2	2.13	0.47
1:D:148:ASP:HB3	1:D:150:THR:CB	2.41	0.47
1:G:391:SER:O	1:G:395:LYS:HG3	2.15	0.47
1:J:361:LYS:O	1:J:362:SER:HB3	2.14	0.47
1:A:451:SER:O	1:A:452:SER:HB3	2.14	0.47
3:I:1437:VAL:HG12	1:J:243:VAL:CG1	2.45	0.47
1:G:30:GLN:HG3	1:G:34:ARG:HD2	1.97	0.47
1:G:33:THR:HG22	1:G:34:ARG:HG3	1.96	0.47
2:K:1060:PRO:HG3	2:K:1080:HIS:CG	2.49	0.47
1:G:396:SER:HB2	1:G:401:ASP:O	2.15	0.47
1:J:7:LEU:N	1:J:431:TRP:CZ3	2.82	0.47
1:A:33:THR:HG22	1:A:34:ARG:HG3	1.96	0.47
1:A:37:PHE:HE1	1:A:440:MSE:HE1	1.78	0.47
1:A:396:SER:HB2	1:A:401:ASP:O	2.14	0.47
1:G:137:TYR:CE2	1:G:138:ARG:HG3	2.49	0.47
1:G:328:PHE:HB2	1:G:351:ILE:HD11	1.97	0.47
1:G:393:LEU:O	1:G:397:ILE:HG13	2.14	0.47
1:J:446:THR:HG22	1:J:447:PHE:N	2.29	0.47
1:A:148:ASP:HB3	1:A:150:THR:CB	2.42	0.47
1:D:396:SER:HB2	1:D:401:ASP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:167:ASN:O	1:J:178:ARG:NH1	2.46	0.47
1:J:37:PHE:CE1	1:J:440:MSE:HE1	2.43	0.47
1:A:240:THR:O	1:A:241:THR:C	2.54	0.47
1:D:37:PHE:HE1	1:D:440:MSE:CE	2.28	0.47
1:G:173:PHE:HZ	2:H:1109:ALA:O	1.97	0.47
1:D:388:SER:OG	1:D:413:LYS:HE3	2.15	0.46
1:G:30:GLN:CD	1:G:34:ARG:HD2	2.36	0.46
1:G:45:TRP:CE2	1:G:55:HIS:HB2	2.50	0.46
1:J:45:TRP:CZ2	1:J:94:PRO:HB2	2.50	0.46
1:J:380:ILE:CG2	1:J:382:GLN:HG3	2.45	0.46
1:A:422:ARG:O	1:A:424:PRO:N	2.48	0.46
1:D:198:ASN:O	1:D:203:GLY:HA2	2.15	0.46
3:F:1434:PHE:O	3:F:1436:VAL:N	2.49	0.46
1:G:343:VAL:HG11	2:H:1066:ARG:CZ	2.45	0.46
1:G:352:GLU:CG	1:G:353:ARG:N	2.78	0.46
1:G:422:ARG:CG	1:G:442:ASN:HD21	2.26	0.46
1:J:352:GLU:CG	1:J:353:ARG:N	2.78	0.46
2:K:1034:TYR:CE2	2:K:1041:PRO:HG2	2.51	0.46
1:D:9:ALA:O	1:D:10:LEU:O	2.33	0.46
1:G:198:ASN:O	1:G:203:GLY:HA2	2.15	0.46
1:G:343:VAL:O	1:G:344:TYR:CB	2.62	0.46
1:G:361:LYS:O	1:G:362:SER:HB3	2.15	0.46
1:J:45:TRP:CE2	1:J:55:HIS:HB2	2.50	0.46
1:G:212:LEU:HD13	1:G:272:ILE:HD13	1.98	0.46
2:H:1001:GLY:CA	2:H:1056:PHE:CE2	2.96	0.46
1:D:321:ASP:OD2	1:D:323:SER:HB2	2.15	0.46
1:G:133:HIS:CE1	1:G:213:PRO:HD3	2.50	0.46
1:G:392:THR:CG2	1:G:408:LEU:HD11	2.44	0.46
1:A:380:ILE:CG2	1:A:382:GLN:HG3	2.45	0.46
2:B:972:ILE:HD11	2:B:1019:LEU:CB	2.43	0.46
1:G:61:ARG:NH1	1:G:107:ASP:OD1	2.49	0.46
1:D:50:THR:HG22	1:D:51:ASP:OD1	2.15	0.46
1:D:251:LYS:NZ	4:D:6119:PGE:O2	2.45	0.46
2:H:1007:GLU:CD	2:H:1049:VAL:HG22	2.36	0.46
2:H:1018:SER:HB3	2:H:1023:ILE:HG13	1.96	0.46
2:B:1060:PRO:HG3	2:B:1080:HIS:CG	2.50	0.46
1:D:273:GLN:OE1	1:D:276:TYR:HE1	1.98	0.46
1:D:352:GLU:CG	1:D:353:ARG:N	2.78	0.46
1:D:289:PRO:HD2	1:D:350:LEU:HB3	1.98	0.46
2:E:1090:SER:HB3	2:E:1104:PHE:CD2	2.51	0.46
1:G:120:GLU:H	1:G:120:GLU:HG3	1.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1040:ARG:N	2:H:1041:PRO:HD3	2.30	0.46
2:H:1060:PRO:HG3	2:H:1080:HIS:CG	2.51	0.46
2:K:1030:THR:HG22	2:K:1031:CYS:N	2.31	0.46
1:A:212:LEU:HD13	1:A:272:ILE:HD13	1.98	0.45
1:J:388:SER:OG	1:J:413:LYS:HE3	2.16	0.45
1:A:402:LEU:HD21	3:C:1448:GLN:CB	2.46	0.45
2:E:1087:ASN:HB3	2:E:1090:SER:HB2	1.99	0.45
1:G:446:THR:HG22	1:G:447:PHE:N	2.30	0.45
1:D:380:ILE:CG2	1:D:382:GLN:HG3	2.47	0.45
1:D:422:ARG:O	1:D:424:PRO:N	2.50	0.45
1:J:210:PRO:HB3	1:J:335:MSE:HE3	1.97	0.45
2:K:1018:SER:HB3	2:K:1023:ILE:HG13	1.98	0.45
1:A:45:TRP:CE2	1:A:55:HIS:HB2	2.52	0.45
1:A:137:TYR:CE2	1:A:138:ARG:HG3	2.51	0.45
2:B:972:ILE:HG12	2:B:995:VAL:HG22	1.97	0.45
2:E:1030:THR:HG22	2:E:1031:CYS:N	2.32	0.45
1:G:422:ARG:O	1:G:424:PRO:N	2.49	0.45
1:J:273:GLN:OE1	1:J:276:TYR:HE1	1.99	0.45
1:A:135:LYS:HD2	1:A:191:GLY:HA3	1.98	0.45
1:G:307:ILE:CG2	1:G:394:SER:HB3	2.47	0.45
1:J:198:ASN:O	1:J:203:GLY:HA2	2.16	0.45
2:K:1015:PRO:O	2:K:1017:THR:N	2.50	0.45
1:A:325:ILE:O	1:A:325:ILE:HG13	2.15	0.45
2:H:1082:GLU:O	2:H:1086:LYS:HG3	2.17	0.45
1:J:7:LEU:C	1:J:9:ALA:H	2.20	0.45
1:J:30:GLN:HB2	1:J:33:THR:HG22	1.98	0.45
1:J:61:ARG:NH1	1:J:107:ASP:OD1	2.49	0.45
1:J:189:LYS:HG2	1:J:304:THR:HG21	1.95	0.45
1:A:352:GLU:CG	1:A:353:ARG:N	2.79	0.45
1:A:368:GLU:HG2	1:A:428:TYR:CE2	2.51	0.45
2:B:1040:ARG:N	2:B:1041:PRO:CD	2.80	0.45
1:G:173:PHE:CE2	2:H:1033:ILE:HD12	2.45	0.45
2:H:1041:PRO:HB2	2:H:1048:ASN:HB2	1.99	0.45
1:J:321:ASP:CG	1:J:323:SER:HB2	2.37	0.45
1:J:422:ARG:O	1:J:424:PRO:N	2.49	0.45
2:K:1037:LEU:H	2:K:1038:PRO:HD3	1.80	0.45
1:D:255:PHE:HB2	4:D:6119:PGE:H6	1.98	0.45
1:J:343:VAL:O	1:J:344:TYR:CB	2.64	0.45
2:B:1009:VAL:HG13	2:B:1046:GLY:O	2.17	0.45
1:D:361:LYS:O	1:D:362:SER:HB3	2.16	0.45
1:D:368:GLU:HG2	1:D:428:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:212:LEU:HD13	1:J:272:ILE:HD13	1.98	0.45
1:J:307:ILE:CG2	1:J:394:SER:HB3	2.47	0.45
1:A:15:ALA:HB2	1:A:24:ARG:NH2	2.31	0.45
1:A:307:ILE:HG12	1:A:390:ALA:HB1	1.98	0.45
1:D:202:GLY:HA2	2:E:1079:ARG:NH1	2.32	0.45
1:J:82:LEU:HD12	1:J:82:LEU:H	1.81	0.45
1:J:210:PRO:HG3	1:J:335:MSE:CE	2.42	0.45
1:J:396:SER:HB2	1:J:401:ASP:O	2.17	0.45
2:K:972:ILE:HG12	2:K:995:VAL:HG22	1.99	0.44
1:D:392:THR:CG2	1:D:408:LEU:HD11	2.42	0.44
1:G:189:LYS:HG2	1:G:304:THR:HG21	1.95	0.44
2:H:972:ILE:HD11	2:H:1019:LEU:CB	2.43	0.44
1:A:328:PHE:HB2	1:A:351:ILE:HD11	1.99	0.44
2:H:1029:LYS:HE2	2:H:1058:CYS:HA	2.00	0.44
2:H:1030:THR:HG22	2:H:1031:CYS:N	2.31	0.44
1:J:30:GLN:HG3	1:J:34:ARG:HD2	2.00	0.44
1:D:30:GLN:CG	1:D:34:ARG:HD2	2.47	0.44
1:G:239:SER:C	1:G:241:THR:H	2.21	0.44
1:J:199:THR:O	1:J:199:THR:CG2	2.64	0.44
2:K:1060:PRO:HG3	2:K:1080:HIS:CD2	2.53	0.44
1:D:307:ILE:CG2	1:D:394:SER:HB3	2.48	0.44
1:G:380:ILE:CG2	1:G:382:GLN:HG3	2.48	0.44
1:J:368:GLU:HG2	1:J:428:TYR:CE2	2.52	0.44
1:J:380:ILE:HG21	1:J:382:GLN:HG3	2.00	0.44
1:D:188:SER:HB3	1:D:190:ASP:OD1	2.18	0.44
1:G:148:ASP:HB3	1:G:150:THR:CB	2.43	0.44
1:G:288:ASN:O	1:G:349:VAL:HA	2.18	0.44
1:G:321:ASP:OD2	1:G:323:SER:HB2	2.16	0.44
1:J:30:GLN:CD	1:J:34:ARG:HD2	2.38	0.44
2:B:1034:TYR:CE2	2:B:1041:PRO:HG2	2.52	0.44
1:D:167:ASN:O	1:D:178:ARG:NH1	2.51	0.44
1:D:291:PRO:HB2	1:D:294:LEU:HD12	2.00	0.44
1:D:391:SER:O	1:D:395:LYS:HG3	2.17	0.44
1:A:78:ASP:O	1:A:79:LEU:HD23	2.18	0.44
1:A:210:PRO:HB3	1:A:335:MSE:HE3	1.99	0.44
1:A:273:GLN:OE1	1:A:276:TYR:HE1	2.00	0.44
3:C:1450:GLY:O	3:C:1454:LYS:HG3	2.18	0.44
1:D:102:ASP:HB3	1:D:105:ILE:H	1.82	0.44
2:E:1049:VAL:HG13	2:E:1050:ARG:N	2.33	0.44
2:E:1060:PRO:HG3	2:E:1080:HIS:CG	2.52	0.44
1:G:368:GLU:HG2	1:G:428:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:THR:O	1:A:199:THR:CG2	2.65	0.43
1:D:30:GLN:HG3	1:D:34:ARG:HD2	2.00	0.43
1:D:61:ARG:NH1	1:D:107:ASP:OD1	2.49	0.43
1:J:102:ASP:HB3	1:J:105:ILE:H	1.83	0.43
1:A:30:GLN:CG	1:A:34:ARG:HD2	2.48	0.43
1:G:210:PRO:CB	1:G:335:MSE:HE3	2.48	0.43
1:A:133:HIS:CE1	1:A:213:PRO:HD3	2.54	0.43
2:B:1030:THR:HG22	2:B:1031:CYS:N	2.33	0.43
1:D:358:ARG:NH2	1:D:380:ILE:HD12	2.33	0.43
1:G:229:LYS:HE3	1:G:332:GLU:CD	2.39	0.43
1:A:381:ILE:O	1:A:417:ILE:HB	2.18	0.43
1:D:172:SER:HB3	2:E:1030:THR:HG23	1.98	0.43
2:K:1079:ARG:O	2:K:1083:ARG:HG2	2.19	0.43
1:A:189:LYS:HG2	1:A:304:THR:HG21	1.97	0.43
1:A:391:SER:O	1:A:395:LYS:HG3	2.18	0.43
1:G:289:PRO:HD2	1:G:350:LEU:HB3	2.00	0.43
2:H:1060:PRO:HG3	2:H:1080:HIS:CD2	2.53	0.43
1:J:133:HIS:CE1	1:J:213:PRO:HD3	2.54	0.43
1:J:307:ILE:HG12	1:J:390:ALA:HB1	2.01	0.43
1:A:361:LYS:O	1:A:362:SER:HB3	2.18	0.43
1:D:288:ASN:O	1:D:349:VAL:HA	2.19	0.43
1:G:199:THR:O	1:G:199:THR:CG2	2.65	0.43
1:G:381:ILE:O	1:G:417:ILE:HB	2.17	0.43
2:H:1047:ILE:HG22	2:H:1047:ILE:O	2.19	0.43
2:B:1015:PRO:O	2:B:1017:THR:N	2.51	0.43
2:B:1060:PRO:HG3	2:B:1080:HIS:CD2	2.54	0.43
1:J:291:PRO:HB2	1:J:294:LEU:HD12	2.00	0.43
2:E:968:GLU:H	2:E:968:GLU:HG3	1.45	0.43
1:G:102:ASP:HB3	1:G:105:ILE:H	1.84	0.43
1:A:316:CYS:SG	1:A:324:LEU:HG	2.59	0.43
1:J:247:ARG:NH1	1:J:338:ASP:OD2	2.49	0.43
2:K:1036:ASN:O	2:K:1037:LEU:HB2	2.19	0.43
2:K:1047:ILE:O	2:K:1047:ILE:HG22	2.19	0.43
1:A:380:ILE:HG21	1:A:382:GLN:HG3	2.00	0.43
1:D:213:PRO:O	1:D:277:ARG:HD3	2.18	0.43
1:G:168:LYS:O	1:G:178:ARG:HD3	2.19	0.43
2:H:1006:LEU:HD21	2:H:1052:ARG:NH1	2.34	0.43
2:H:1079:ARG:O	2:H:1083:ARG:HG2	2.18	0.43
3:I:1452:PHE:C	3:I:1452:PHE:CD1	2.92	0.43
1:J:328:PHE:HB2	1:J:351:ILE:HD11	2.01	0.43
1:J:386:PHE:HB2	1:J:389:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ILE:CG2	1:A:394:SER:HB3	2.49	0.42
2:E:966:MSE:HE2	2:E:1020:GLY:CA	2.49	0.42
1:J:381:ILE:O	1:J:417:ILE:HB	2.18	0.42
1:A:102:ASP:HB3	1:A:105:ILE:H	1.84	0.42
1:A:212:LEU:O	1:A:277:ARG:HD2	2.18	0.42
1:A:321:ASP:OD2	1:A:353:ARG:NH2	2.52	0.42
1:D:10:LEU:HA	1:D:11:PRO:HD3	1.93	0.42
1:D:199:THR:O	1:D:200:THR:C	2.56	0.42
1:D:210:PRO:HB3	1:D:335:MSE:HE3	1.99	0.42
1:D:307:ILE:HG12	1:D:390:ALA:HB1	2.01	0.42
1:D:328:PHE:HB2	1:D:351:ILE:HD11	2.01	0.42
1:J:159:SER:C	1:J:161:GLU:H	2.22	0.42
1:J:238:ASP:OD2	1:J:240:THR:CB	2.68	0.42
1:J:451:SER:O	1:J:452:SER:CB	2.67	0.42
3:L:1452:PHE:CD1	3:L:1452:PHE:C	2.92	0.42
1:D:274:LYS:HG3	1:D:275:GLU:OE2	2.20	0.42
2:E:972:ILE:HG12	2:E:995:VAL:HG22	1.99	0.42
2:E:1037:LEU:N	2:E:1038:PRO:CD	2.82	0.42
1:G:252:GLN:HG3	1:G:335:MSE:SE	2.69	0.42
1:J:440:MSE:HE2	1:J:440:MSE:HB2	1.98	0.42
1:A:168:LYS:O	1:A:178:ARG:HD3	2.19	0.42
1:A:188:SER:HB3	1:A:190:ASP:OD1	2.20	0.42
3:C:1452:PHE:CD1	3:C:1452:PHE:C	2.92	0.42
1:D:135:LYS:HD2	1:D:191:GLY:HA3	2.01	0.42
1:D:316:CYS:SG	1:D:324:LEU:HG	2.59	0.42
1:G:247:ARG:NH1	1:G:338:ASP:OD2	2.50	0.42
1:J:148:ASP:HB3	1:J:150:THR:CB	2.43	0.42
1:J:358:ARG:NH2	1:J:380:ILE:HD12	2.33	0.42
2:K:1065:THR:HG22	2:K:1067:LYS:CG	2.49	0.42
1:D:159:SER:C	1:D:161:GLU:H	2.23	0.42
1:J:135:LYS:HD2	1:J:191:GLY:HA3	2.02	0.42
1:A:120:GLU:H	1:A:120:GLU:HG3	1.47	0.42
1:D:276:TYR:CD2	4:D:6119:PGE:H5	2.53	0.42
2:E:1079:ARG:O	2:E:1083:ARG:HG2	2.20	0.42
3:F:1434:PHE:C	3:F:1436:VAL:H	2.23	0.42
1:J:199:THR:O	1:J:200:THR:C	2.58	0.42
1:A:358:ARG:NH2	1:A:380:ILE:HD12	2.34	0.42
1:D:199:THR:O	1:D:199:THR:CG2	2.68	0.42
1:G:386:PHE:HB2	1:G:389:TRP:CE2	2.54	0.42
1:J:50:THR:HG22	1:J:51:ASP:OD1	2.20	0.42
1:A:290:PHE:HA	1:A:291:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:ILE:HG13	1:D:325:ILE:O	2.18	0.42
2:E:1010:ASP:HB3	2:E:1046:GLY:HA2	2.02	0.42
3:F:1450:GLY:O	3:F:1454:LYS:HG3	2.20	0.42
2:E:972:ILE:CG2	2:E:973:SER:N	2.83	0.42
2:E:1015:PRO:O	2:E:1017:THR:N	2.52	0.42
1:G:28:SER:HA	1:G:34:ARG:O	2.19	0.42
1:G:82:LEU:HD12	1:G:82:LEU:H	1.84	0.42
1:J:28:SER:HA	1:J:34:ARG:O	2.19	0.42
1:J:343:VAL:CG1	2:K:1066:ARG:CZ	2.95	0.42
1:A:213:PRO:O	1:A:277:ARG:HD3	2.19	0.42
1:A:239:SER:HA	1:A:246:LYS:NZ	2.34	0.42
1:A:288:ASN:O	1:A:349:VAL:HA	2.20	0.42
1:D:10:LEU:HG	1:D:11:PRO:HD2	2.02	0.42
1:D:43:ILE:O	1:D:56:SER:HA	2.19	0.42
1:G:358:ARG:NH2	1:G:380:ILE:HD12	2.34	0.42
2:H:972:ILE:HG12	2:H:995:VAL:HG22	2.02	0.42
2:K:972:ILE:CG2	2:K:973:SER:N	2.82	0.42
1:A:50:THR:HG22	1:A:51:ASP:OD1	2.19	0.41
1:D:380:ILE:HG21	1:D:382:GLN:HG3	2.01	0.41
1:G:332:GLU:HG2	3:I:1443:MSE:HE3	2.02	0.41
1:G:451:SER:O	1:G:452:SER:CB	2.67	0.41
1:J:168:LYS:O	1:J:178:ARG:HD3	2.20	0.41
1:A:15:ALA:HB2	1:A:39:GLN:OE1	2.19	0.41
2:B:1061:VAL:CG1	2:B:1066:ARG:HA	2.51	0.41
2:B:1065:THR:HG22	2:B:1067:LYS:CG	2.49	0.41
2:B:1079:ARG:O	2:B:1083:ARG:HG2	2.20	0.41
3:C:1437:VAL:O	3:C:1441:LEU:HG	2.21	0.41
1:G:50:THR:HG22	1:G:51:ASP:OD1	2.21	0.41
2:H:1054:THR:HG23	2:H:1103:VAL:HG22	2.01	0.41
1:J:33:THR:HG22	1:J:34:ARG:HG3	2.01	0.41
1:A:159:SER:C	1:A:161:GLU:H	2.24	0.41
1:G:210:PRO:HB2	1:G:212:LEU:HG	2.02	0.41
1:G:380:ILE:HG21	1:G:382:GLN:HG3	2.02	0.41
1:A:252:GLN:HG3	1:A:335:MSE:SE	2.70	0.41
2:B:966:MSE:HE2	2:B:1020:GLY:CA	2.50	0.41
1:D:451:SER:O	1:D:452:SER:CB	2.68	0.41
2:E:1006:LEU:HD21	2:E:1052:ARG:NH1	2.35	0.41
2:E:1039:ASN:O	2:E:1040:ARG:C	2.58	0.41
1:G:159:SER:C	1:G:161:GLU:H	2.22	0.41
2:H:966:MSE:HE2	2:H:1020:GLY:CA	2.51	0.41
1:J:213:PRO:O	1:J:277:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:966:MSE:HE2	2:K:1020:GLY:CA	2.50	0.41
1:A:302:ILE:HA	1:A:316:CYS:O	2.21	0.41
1:D:381:ILE:O	1:D:417:ILE:HB	2.20	0.41
1:G:30:GLN:HB2	1:G:33:THR:HG22	2.02	0.41
1:G:189:LYS:NZ	1:G:304:THR:HG22	2.36	0.41
1:G:210:PRO:CD	1:G:335:MSE:HE3	2.50	0.41
1:G:440:MSE:HE2	1:G:440:MSE:HB2	2.00	0.41
2:H:1067:LYS:HA	2:H:1068:PRO:HD3	1.90	0.41
1:J:7:LEU:HB2	1:J:431:TRP:CE3	2.55	0.41
1:D:137:TYR:CD2	1:D:138:ARG:HG3	2.56	0.41
2:E:1061:VAL:CG1	2:E:1066:ARG:HA	2.51	0.41
1:G:43:ILE:O	1:G:56:SER:HA	2.20	0.41
1:G:212:LEU:O	1:G:277:ARG:HD2	2.21	0.41
2:H:1030:THR:CG2	2:H:1031:CYS:N	2.83	0.41
1:J:252:GLN:HG3	1:J:335:MSE:SE	2.71	0.41
1:D:252:GLN:HG3	1:D:335:MSE:SE	2.71	0.41
2:E:1060:PRO:HG3	2:E:1080:HIS:CD2	2.56	0.41
1:G:133:HIS:HA	1:G:134:PRO:HD3	1.93	0.41
1:J:93:VAL:HA	1:J:94:PRO:HD3	1.90	0.41
1:A:7:LEU:HG	1:A:9:ALA:HB3	2.02	0.41
1:A:30:GLN:CD	1:A:34:ARG:HD2	2.40	0.41
2:B:972:ILE:CG2	2:B:973:SER:N	2.83	0.41
1:D:386:PHE:HB2	1:D:389:TRP:CE2	2.55	0.41
2:E:1030:THR:CG2	2:E:1031:CYS:N	2.84	0.41
2:E:1084:LEU:C	2:E:1086:LYS:H	2.23	0.41
1:G:179:VAL:HG21	1:G:281:VAL:HG11	2.01	0.41
1:G:321:ASP:OD2	1:G:353:ARG:NH2	2.54	0.41
1:G:402:LEU:HD21	3:I:1448:GLN:CB	2.50	0.41
2:H:1015:PRO:O	2:H:1017:THR:N	2.54	0.41
1:J:288:ASN:O	1:J:349:VAL:HA	2.21	0.41
1:J:289:PRO:HD2	1:J:350:LEU:HB3	2.02	0.41
1:J:386:PHE:HB2	1:J:389:TRP:CZ2	2.55	0.41
1:A:239:SER:HA	1:A:246:LYS:HZ1	1.86	0.41
1:A:291:PRO:HB2	1:A:294:LEU:HD12	2.03	0.41
1:A:451:SER:O	1:A:452:SER:CB	2.68	0.41
1:D:444:THR:CG2	1:D:445:LEU:N	2.74	0.41
3:F:1452:PHE:CD1	3:F:1452:PHE:C	2.93	0.41
2:H:1000:TYR:C	2:H:1056:PHE:HD2	2.22	0.41
1:J:26:ILE:HB	1:J:440:MSE:HE3	2.03	0.41
1:J:133:HIS:HA	1:J:134:PRO:HD3	1.92	0.41
1:J:332:GLU:HG2	3:L:1443:MSE:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1030:THR:CG2	2:K:1031:CYS:N	2.82	0.41
2:K:1087:ASN:O	2:K:1087:ASN:CG	2.60	0.41
1:D:168:LYS:O	1:D:178:ARG:HD3	2.21	0.41
1:D:240:THR:OG1	1:G:9:ALA:HB2	2.21	0.41
1:D:386:PHE:HB2	1:D:389:TRP:CZ2	2.56	0.41
1:G:290:PHE:HA	1:G:291:PRO:HD3	1.86	0.41
1:G:291:PRO:HB2	1:G:294:LEU:HD12	2.02	0.41
1:J:137:TYR:CD2	1:J:138:ARG:HG3	2.56	0.41
1:J:274:LYS:HG3	1:J:275:GLU:OE2	2.20	0.41
2:K:1054:THR:HG23	2:K:1103:VAL:HG22	2.03	0.41
1:A:372:LYS:HE2	1:A:385:ASN:HD21	1.84	0.40
1:D:251:LYS:HB3	4:D:6119:PGE:H62	2.03	0.40
1:G:135:LYS:HD2	1:G:191:GLY:HA3	2.03	0.40
1:G:316:CYS:SG	1:G:324:LEU:HG	2.61	0.40
1:J:210:PRO:HB2	1:J:212:LEU:HG	2.03	0.40
1:A:228:ASN:ND2	3:C:1435:LYS:HB2	2.36	0.40
2:B:1047:ILE:O	2:B:1047:ILE:HG22	2.20	0.40
2:E:1036:ASN:O	2:E:1037:LEU:HB2	2.21	0.40
1:G:321:ASP:CG	1:G:323:SER:HB2	2.41	0.40
1:G:386:PHE:HB2	1:G:389:TRP:CZ2	2.55	0.40
2:H:966:MSE:HG3	2:H:1020:GLY:CA	2.50	0.40
1:J:302:ILE:HA	1:J:316:CYS:O	2.21	0.40
1:J:321:ASP:OD2	1:J:353:ARG:NH2	2.54	0.40
1:A:321:ASP:CG	1:A:323:SER:HB2	2.41	0.40
2:B:1038:PRO:C	2:B:1040:ARG:H	2.24	0.40
1:D:179:VAL:HG21	1:D:281:VAL:HG11	2.04	0.40
2:E:1047:ILE:O	2:E:1047:ILE:HG22	2.20	0.40
1:J:290:PHE:HA	1:J:291:PRO:HD3	1.85	0.40
2:K:988:ARG:HA	2:K:1010:ASP:HA	2.02	0.40
2:H:1061:VAL:CG1	2:H:1066:ARG:HA	2.52	0.40
1:J:343:VAL:HG12	1:J:344:TYR:N	2.36	0.40
2:K:1087:ASN:N	2:K:1088:PRO:HD3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	432/452 (96%)	396 (92%)	32 (7%)	4 (1%)	14	31
1	D	431/452 (95%)	397 (92%)	29 (7%)	5 (1%)	11	24
1	G	432/452 (96%)	396 (92%)	32 (7%)	4 (1%)	14	31
1	J	433/452 (96%)	399 (92%)	29 (7%)	5 (1%)	11	24
2	B	144/148 (97%)	120 (83%)	19 (13%)	5 (4%)	3	4
2	E	144/148 (97%)	117 (81%)	20 (14%)	7 (5%)	2	2
2	H	144/148 (97%)	121 (84%)	19 (13%)	4 (3%)	4	7
2	K	144/148 (97%)	120 (83%)	19 (13%)	5 (4%)	3	4
3	C	24/36 (67%)	21 (88%)	2 (8%)	1 (4%)	2	3
3	F	24/36 (67%)	21 (88%)	3 (12%)	0	100	100
3	I	26/36 (72%)	25 (96%)	1 (4%)	0	100	100
3	L	22/36 (61%)	21 (96%)	1 (4%)	0	100	100
All	All	2400/2544 (94%)	2154 (90%)	206 (9%)	40 (2%)	7	16

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	TYR
2	B	1036	ASN
3	C	1435	LYS
1	D	344	TYR
1	G	344	TYR
1	J	344	TYR
2	B	1016	LEU
2	E	1016	LEU
1	G	339	VAL
2	H	1016	LEU
1	J	339	VAL
2	K	1016	LEU
1	A	339	VAL
2	B	975	SER
1	D	339	VAL
2	E	975	SER
2	E	1040	ARG
2	H	975	SER

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Mol	Chain	Res	Type
2	K	975	SER
2	K	1036	ASN
1	A	200	THR
1	D	10	LEU
2	H	1036	ASN
2	B	1087	ASN
1	D	200	THR
1	J	200	THR
2	E	1036	ASN
2	E	1038	PRO
2	E	1088	PRO
1	G	200	THR
2	K	1046	GLY
2	B	1046	GLY
2	E	1046	GLY
2	H	1046	GLY
1	A	423	ILE
1	G	423	ILE
1	J	12	ILE
1	J	423	ILE
2	K	1087	ASN
1	D	423	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/415 (99%)	396 (96%)	15 (4%)	30	56
1	D	410/415 (99%)	398 (97%)	12 (3%)	37	64
1	G	411/415 (99%)	398 (97%)	13 (3%)	34	60
1	J	412/415 (99%)	400 (97%)	12 (3%)	37	64
2	B	132/133 (99%)	128 (97%)	4 (3%)	36	63
2	E	132/133 (99%)	128 (97%)	4 (3%)	36	63
2	H	132/133 (99%)	128 (97%)	4 (3%)	36	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	132/133 (99%)	128 (97%)	4 (3%)	36	63
3	C	22/28 (79%)	22 (100%)	0	100	100
3	F	22/28 (79%)	21 (96%)	1 (4%)	23	47
3	I	24/28 (86%)	22 (92%)	2 (8%)	9	19
3	L	21/28 (75%)	21 (100%)	0	100	100
All	All	2261/2304 (98%)	2190 (97%)	71 (3%)	35	62

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	29	SER
1	A	33	THR
1	A	101	GLU
1	A	102	ASP
1	A	120	GLU
1	A	148	ASP
1	A	176	ASP
1	A	185	LEU
1	A	198	ASN
1	A	210	PRO
1	A	217	LEU
1	A	281	VAL
1	A	286	THR
1	A	433	ASP
2	B	968	GLU
2	B	1049	VAL
2	B	1079	ARG
2	B	1098	ASP
1	D	29	SER
1	D	33	THR
1	D	101	GLU
1	D	102	ASP
1	D	120	GLU
1	D	148	ASP
1	D	185	LEU
1	D	198	ASN
1	D	210	PRO
1	D	217	LEU
1	D	281	VAL

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Mol	Chain	Res	Type
1	D	286	THR
2	E	968	GLU
2	E	1049	VAL
2	E	1079	ARG
2	E	1098	ASP
3	F	1434	PHE
1	G	29	SER
1	G	33	THR
1	G	101	GLU
1	G	102	ASP
1	G	120	GLU
1	G	148	ASP
1	G	176	ASP
1	G	185	LEU
1	G	198	ASN
1	G	210	PRO
1	G	217	LEU
1	G	281	VAL
1	G	286	THR
2	H	968	GLU
2	H	1049	VAL
2	H	1079	ARG
2	H	1098	ASP
3	I	1430	ASP
3	I	1456	LEU
1	J	29	SER
1	J	33	THR
1	J	101	GLU
1	J	102	ASP
1	J	120	GLU
1	J	148	ASP
1	J	176	ASP
1	J	185	LEU
1	J	210	PRO
1	J	217	LEU
1	J	281	VAL
1	J	286	THR
2	K	968	GLU
2	K	1049	VAL
2	K	1079	ARG
2	K	1098	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	A	430	ASN
2	B	967	ASN
2	B	969	ASN
2	B	1075	GLN
2	B	1087	ASN
1	D	262	ASN
1	D	430	ASN
2	E	967	ASN
2	E	969	ASN
2	E	1075	GLN
3	F	1457	ASN
1	G	262	ASN
2	H	967	ASN
2	H	969	ASN
3	I	1448	GLN
1	J	262	ASN
2	K	967	ASN
2	K	969	ASN
2	K	1075	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PGE	D	6119	-	9,9,9	0.93	1 (11%)	8,8,8	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	D	6119	-	-	1/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6119	PGE	C5-C6	2.25	1.61	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	6119	PGE	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	6119	PGE	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	431/452 (95%)	0.58	20 (4%) 38 32	44, 65, 96, 118	0
1	D	430/452 (95%)	0.52	19 (4%) 39 33	41, 65, 98, 118	0
1	G	431/452 (95%)	0.53	19 (4%) 39 33	43, 65, 97, 117	0
1	J	432/452 (95%)	0.54	26 (6%) 29 23	41, 64, 99, 117	0
2	B	145/148 (97%)	1.17	23 (15%) 6 5	53, 90, 116, 129	0
2	E	145/148 (97%)	1.32	29 (20%) 3 3	52, 90, 116, 129	0
2	H	145/148 (97%)	1.63	45 (31%) 1 1	58, 94, 119, 144	0
2	K	145/148 (97%)	1.04	20 (13%) 8 6	56, 92, 117, 137	0
3	C	24/36 (66%)	0.75	1 (4%) 41 35	59, 69, 91, 108	0
3	F	24/36 (66%)	0.77	3 (12%) 9 7	58, 69, 89, 109	0
3	I	26/36 (72%)	0.73	1 (3%) 44 38	57, 71, 118, 123	0
3	L	23/36 (63%)	0.61	1 (4%) 40 34	62, 70, 89, 96	0
All	All	2401/2544 (94%)	0.73	207 (8%) 18 15	41, 70, 106, 144	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1076	LEU	5.0
2	H	1019	LEU	5.0
2	H	1038	PRO	4.7
2	B	1076	LEU	4.6
1	G	7	LEU	4.6
1	D	7	LEU	4.5
1	A	175	LEU	4.3
1	A	7	LEU	4.1
1	G	175	LEU	4.1
2	B	1047	ILE	4.1
2	E	1035	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	984	LEU	3.9
2	H	1037	LEU	3.8
1	G	176	ASP	3.8
1	J	23	PRO	3.8
2	H	1044	GLY	3.8
1	A	424	PRO	3.7
1	A	423	ILE	3.7
2	K	1047	ILE	3.7
1	D	318	SER	3.7
2	B	1098	ASP	3.6
2	E	1097	ALA	3.6
3	C	1434	PHE	3.6
1	D	175	LEU	3.5
2	K	1038	PRO	3.5
2	H	1034	TYR	3.5
2	K	984	LEU	3.5
2	H	1032	ILE	3.5
2	H	982	TYR	3.5
2	E	1098	ASP	3.5
2	E	1089	ASN	3.5
2	K	1032	ILE	3.5
2	E	1021	GLY	3.5
1	D	423	ILE	3.4
2	E	1047	ILE	3.4
2	H	987	LEU	3.4
2	H	1035	ALA	3.3
1	J	175	LEU	3.3
2	H	974	PRO	3.2
1	G	423	ILE	3.2
2	E	1022	VAL	3.2
1	G	123	PRO	3.2
2	B	1072	PRO	3.2
1	J	423	ILE	3.2
2	B	972	ILE	3.2
1	A	103	VAL	3.1
1	G	173	PHE	3.1
2	B	1037	LEU	3.1
1	A	123	PRO	3.1
1	J	176	ASP	3.1
2	H	1016	LEU	3.1
2	H	985	LEU	3.1
2	K	1019	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	L	1434	PHE	3.0
1	J	452	SER	3.0
2	E	1072	PRO	3.0
2	H	1017	THR	3.0
1	D	156	ILE	2.9
1	D	380	ILE	2.9
2	H	977	ASP	2.9
2	H	976	LEU	2.9
2	H	1042	LYS	2.9
2	H	979	LEU	2.9
2	B	1097	ALA	2.9
2	K	1049	VAL	2.9
2	K	967	ASN	2.9
2	H	992	HIS	2.9
1	G	400	SER	2.8
2	K	1034	TYR	2.8
3	F	1434	PHE	2.8
1	D	40	ASP	2.8
2	E	1037	LEU	2.8
2	H	970	TYR	2.8
2	K	982	TYR	2.8
2	H	1015	PRO	2.8
1	A	176	ASP	2.8
2	H	1076	LEU	2.8
2	H	1014	ILE	2.8
2	H	1111	GLU	2.8
1	A	23	PRO	2.8
2	E	970	TYR	2.8
2	K	1035	ALA	2.7
2	E	1010	ASP	2.7
1	D	100	VAL	2.7
1	J	109	PHE	2.7
2	E	1046	GLY	2.7
1	D	401	ASP	2.7
2	B	1057	ASN	2.7
2	B	1035	ALA	2.7
1	D	421	GLU	2.7
2	H	1049	VAL	2.7
1	A	431	TRP	2.7
2	H	972	ILE	2.7
1	D	161	GLU	2.6
1	J	123	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	452	SER	2.6
2	B	1024	ILE	2.6
1	J	408	LEU	2.6
2	E	1019	LEU	2.6
1	J	377	SER	2.6
1	A	411	GLU	2.6
3	I	1434	PHE	2.6
2	K	985	LEU	2.5
1	D	15	ALA	2.5
2	H	1081	ILE	2.5
2	H	1023	ILE	2.5
2	H	1030	THR	2.5
2	K	968	GLU	2.5
2	H	1018	SER	2.5
1	D	120	GLU	2.5
2	B	1041	PRO	2.5
1	J	100	VAL	2.5
2	H	971	TYR	2.5
2	B	1074	HIS	2.5
2	K	1111	GLU	2.4
2	K	1037	LEU	2.4
2	H	991	PRO	2.4
2	K	1079	ARG	2.4
2	H	990	VAL	2.4
2	E	1029	LYS	2.4
2	E	1020	GLY	2.4
2	H	1101	THR	2.4
1	J	431	TRP	2.4
2	B	985	LEU	2.4
1	D	23	PRO	2.4
1	G	23	PRO	2.4
1	J	172	SER	2.4
1	J	318	SER	2.4
2	E	1090	SER	2.4
1	J	420	ILE	2.4
2	E	1032	ILE	2.4
2	B	1038	PRO	2.3
2	H	1022	VAL	2.3
2	B	1026	PHE	2.3
2	H	1047	ILE	2.3
2	E	1034	TYR	2.3
1	J	171	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	402	LEU	2.3
2	E	1025	THR	2.3
2	E	1024	ILE	2.3
1	G	172	SER	2.3
2	H	1000	TYR	2.3
2	H	1029	LYS	2.3
2	K	1030	THR	2.3
1	A	450	ILE	2.3
2	E	1033	ILE	2.3
2	H	1024	ILE	2.3
1	D	177	ALA	2.3
2	E	984	LEU	2.3
2	K	1016	LEU	2.3
1	J	170	ASN	2.3
2	E	1075	GLN	2.3
1	G	318	SER	2.3
2	H	984	LEU	2.3
1	J	6	ARG	2.2
1	J	421	GLU	2.2
1	J	434	GLN	2.2
2	H	986	GLN	2.2
2	E	1085	LYS	2.2
1	J	405	LEU	2.2
1	A	401	ASP	2.2
2	K	1033	ILE	2.2
2	E	1005	PHE	2.2
2	E	1009	VAL	2.2
1	G	174	GLY	2.2
1	A	180	ASN	2.2
2	H	994	VAL	2.2
1	J	53	LEU	2.2
2	E	1038	PRO	2.1
2	H	1033	ILE	2.1
3	F	1439	VAL	2.1
2	K	1076	LEU	2.1
1	D	240	THR	2.1
2	B	1071	ASP	2.1
1	J	98	SER	2.1
2	H	973	SER	2.1
1	G	436	ASN	2.1
1	A	433	ASP	2.1
1	A	53	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	177	ALA	2.1
1	A	174	GLY	2.1
2	B	1100	GLY	2.1
1	A	318	SER	2.1
1	A	420	ILE	2.1
1	D	452	SER	2.1
1	G	391	SER	2.1
1	G	450	ILE	2.1
1	G	100	VAL	2.1
2	B	1016	LEU	2.1
1	G	401	ASP	2.1
1	J	234	TYR	2.1
2	B	1085	LYS	2.0
1	J	236	SER	2.0
2	B	1077	VAL	2.0
2	K	1026	PHE	2.0
1	D	53	LEU	2.0
2	H	1011	LEU	2.0
1	D	171	ASN	2.0
2	B	1046	GLY	2.0
1	G	399	GLU	2.0
1	G	443	LYS	2.0
1	J	179	VAL	2.0
1	J	384	VAL	2.0
2	B	1075	GLN	2.0
2	E	985	LEU	2.0
3	F	1457	ASN	2.0
2	H	1059	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PGE	D	6119	10/10	0.80	0.18	70,72,77,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.