



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2025 – 10:34 AM EDT

PDB ID : 9E1J / pdb\_00009e1j  
Title : Alpha-Delta heterodimeric form of soluble hydrogenase I from *Pyrococcus furiosus*. Data processed and model refined in P21221  
Authors : Lanzilotta, W.N.; Adams, M.W.W.  
Deposited on : 2024-10-21  
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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

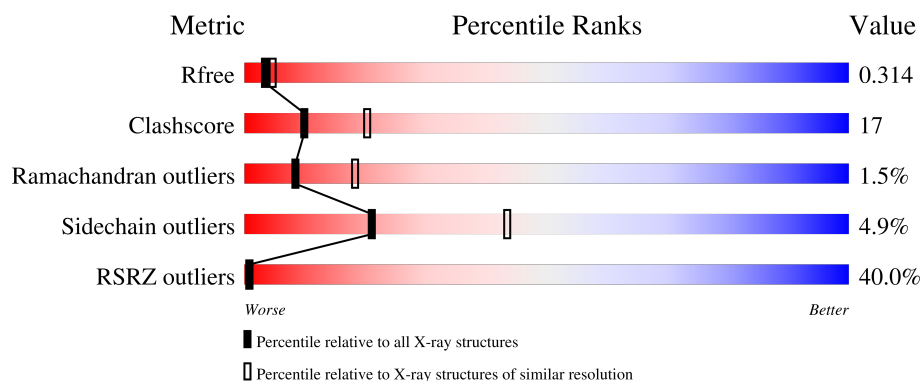
# 1 Overall quality at a glance

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  $\geq 3$ , 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	256	<div> <div>72%</div> <div>27%</div> <div>.</div> </div>
1	C	256	<div> <div>77%</div> <div>58%</div> <div>37%</div> <div>..</div> </div>
2	B	419	<div> <div>2%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
2	D	419	<div> <div>79%</div> <div>57%</div> <div>40%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	A	501	-	-	X	-
3	SF4	C	502	-	-	X	-
4	FCO	B	501	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10787 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 Sulfhydrogenase 1 subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	1	0
			2009	1292	328	369	20			
1	C	254	Total	C	N	O	S	5	0	0
			1987	1276	325	366	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	ALA	LYS	conflict	UNP E7FHU4
A	252	ALA	GLU	conflict	UNP E7FHU4
C	226	ALA	LYS	conflict	UNP E7FHU4
C	252	ALA	GLU	conflict	UNP E7FHU4

- Molecule 2 is a protein called Sulfhydrogenase 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	1	0
			3332	2145	556	616	15			
2	D	419	Total	C	N	O	S	0	0	0
			3324	2140	554	615	15			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula:  $C_3FeN_2O$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ni	0	0
			1	1		
5	D	1	Total	Ni	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

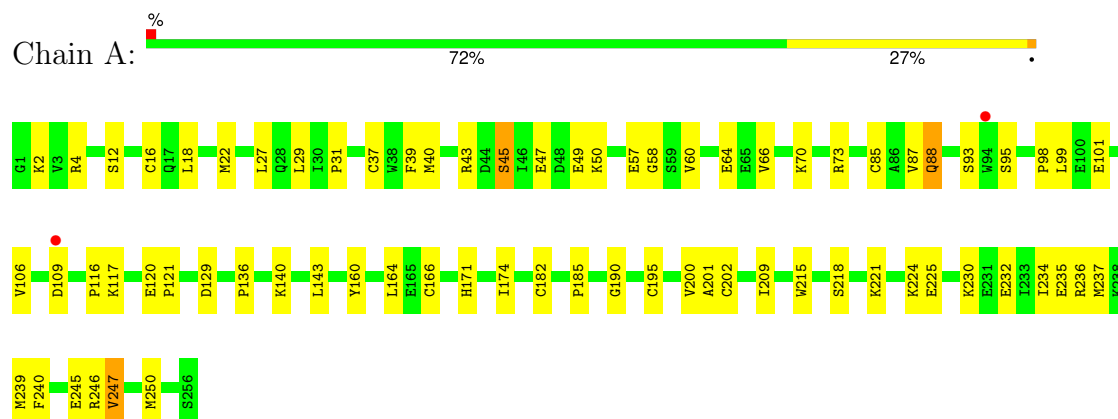
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	31	Total	O	0	0
			31	31		
7	B	30	Total	O	0	0
			30	30		

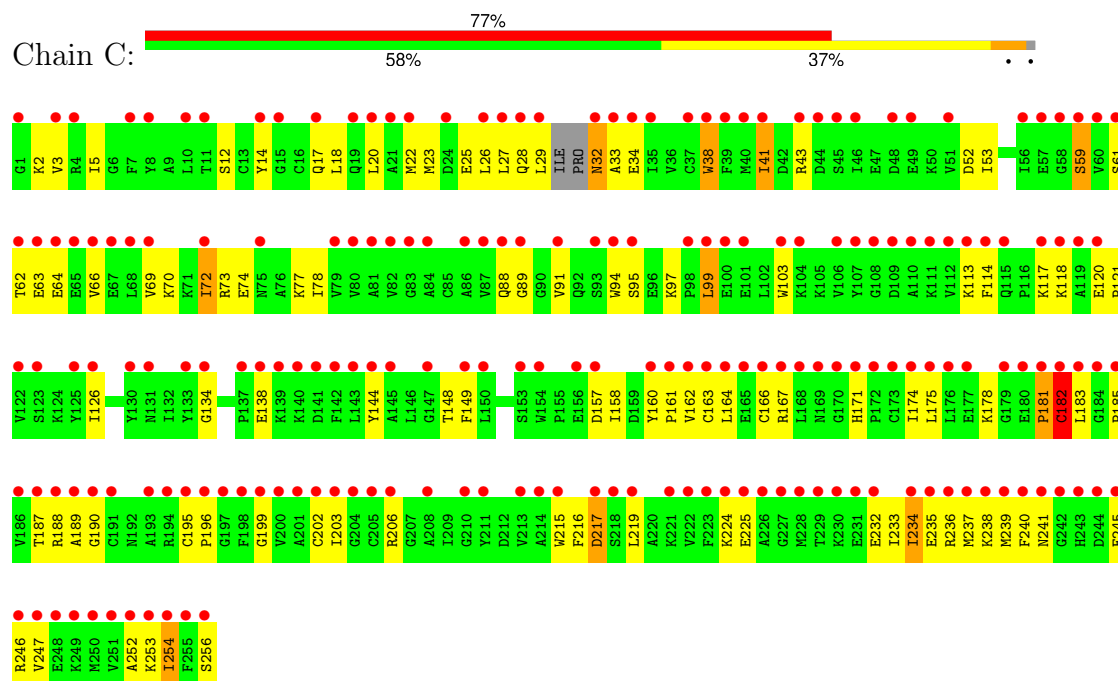
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sulfhydrogenase 1 subunit delta

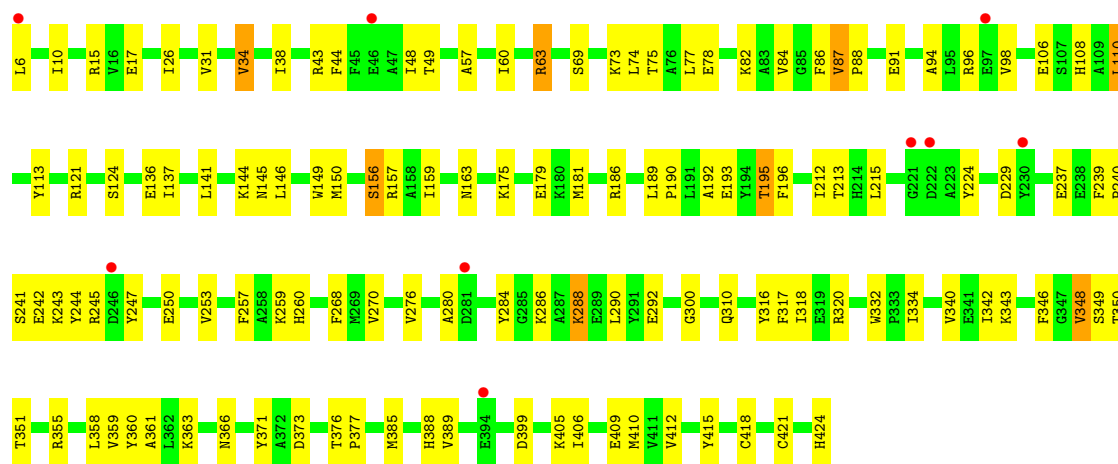


- Molecule 1: Sulfhydrogenase 1 subunit delta

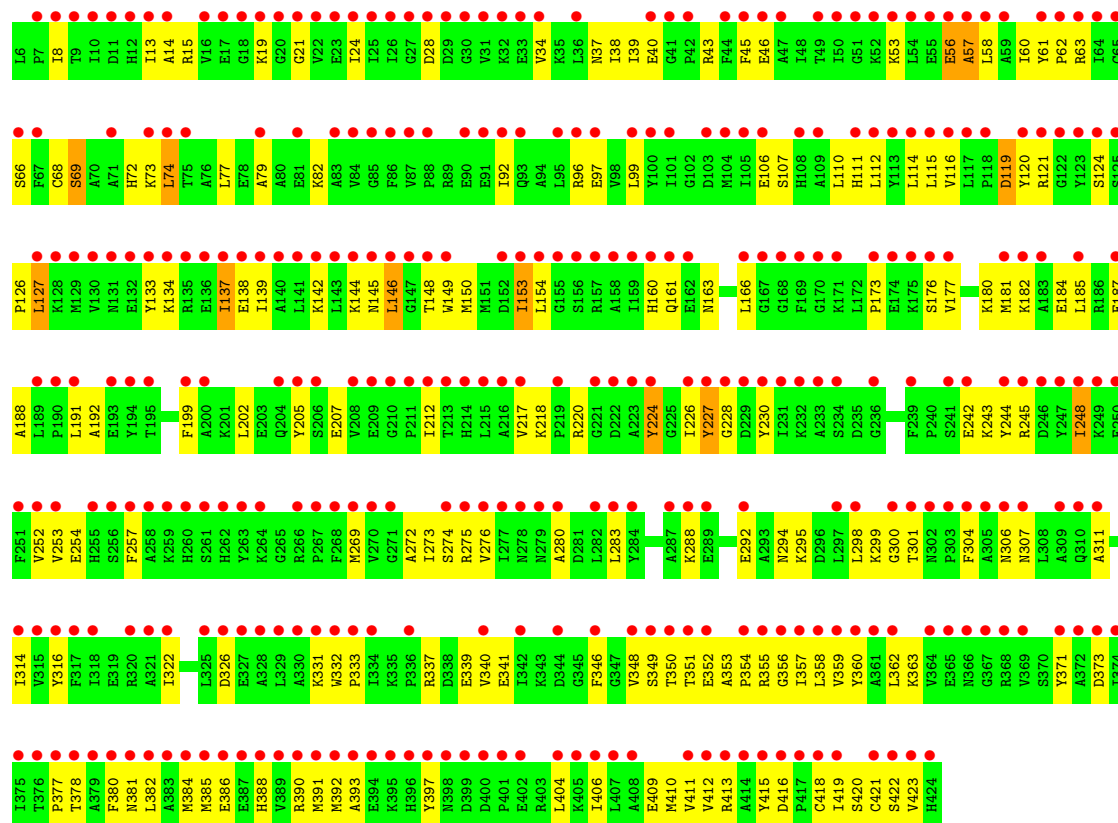
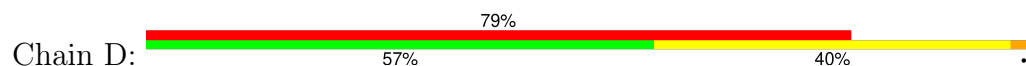


- Molecule 2: Sulfhydrogenase 1 subunit alpha





• Molecule 2: Sulfhydrylase 1 subunit alpha





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.29Å 111.19Å 141.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.91 – 2.60 35.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.91-2.60) 93.3 (35.91-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.86 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.256 , 0.313 0.258 , 0.314	Depositor DCC
$R_{free}$ test set	44333 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.835	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 66.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	10787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4544e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CL, FCO, NI

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	0.53	0/2055	0.73	0/2769
1	C	0.39	0/2028	0.68	0/2732
2	B	0.57	0/3406	0.77	1/4599 (0.0%)
2	D	0.34	0/3394	0.57	0/4584
All	All	0.47	0/10883	0.69	1/14684 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	ARG	CA-C-O	5.08	127.04	118.91

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2009	0	2012	59	0
1	C	1987	0	1980	82	0
2	B	3332	0	3359	93	0
2	D	3324	0	3352	156	0
3	A	24	0	0	4	0
3	C	40	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	0	8	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	1	0	0	0	0
7	A	31	0	0	2	0
7	B	30	0	0	4	0
All	All	10787	0	10703	369	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 17.

All (369) 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)
1:A:239:MET:HG3	2:B:60:ILE:HD11	1.43	1.00
2:B:377:PRO:HD2	4:B:501:FCO:N1	1.80	0.96
1:C:43:ARG:HH12	2:D:406:ILE:HG22	1.31	0.96
2:B:377:PRO:HD2	4:B:501:FCO:C1	1.97	0.94
2:D:19:LYS:HB3	2:D:40:GLU:HG2	1.54	0.89
2:D:275:ARG:HE	2:D:352:GLU:HB3	1.42	0.84
2:D:385:MET:HE1	2:D:412:VAL:HG13	1.62	0.82
2:B:113:TYR:HH	2:B:195:THR:HG1	1.28	0.82
1:A:218:SER:HB3	1:A:221:LYS:HB2	1.64	0.80
1:C:52:ASP:HA	1:C:77:LYS:HG3	1.64	0.79
2:D:57:ALA:HB1	2:D:61:TYR:CZ	2.17	0.79
2:D:110:LEU:HA	2:D:114:LEU:HD23	1.64	0.79
2:D:363:LYS:HB3	2:D:371:TYR:HB3	1.64	0.79
1:C:41:ILE:HD12	2:D:127:LEU:HG	1.65	0.78
1:A:88:GLN:NE2	1:A:240:PHE:O	2.17	0.77
2:D:24:ILE:HG12	2:D:34:VAL:HG12	1.64	0.77
2:B:121:ARG:NH2	2:B:136:GLU:OE2	2.18	0.76
1:A:37:CYS:HA	1:A:45:SER:HB3	1.66	0.76
1:A:29:LEU:HD13	1:A:143:LEU:HD12	1.68	0.74
2:D:166:LEU:HB3	2:D:340:VAL:HG21	1.68	0.73
2:D:107:SER:OG	2:D:355:ARG:NH1	2.19	0.73
2:D:226:ILE:HD13	2:D:352:GLU:HB2	1.69	0.73
2:B:6:LEU:HD23	2:B:26:ILE:HD11	1.71	0.72
2:D:242:GLU:HG3	2:D:348:VAL:HB	1.71	0.72
2:D:177:VAL:HA	2:D:180:LYS:HD3	1.71	0.72
2:D:137:ILE:HG13	2:D:138:GLU:N	2.03	0.72
2:D:21:GLY:O	2:D:37:ASN:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:CYS:HB2	1:C:202:CYS:H	1.55	0.71
1:C:175:LEU:HG	1:C:181:PRO:HA	1.73	0.70
1:A:232:GLU:OE2	1:A:236:ARG:NH1	2.24	0.70
2:D:19:LYS:H	2:D:40:GLU:HG3	1.56	0.70
1:A:245:GLU:CD	1:A:245:GLU:H	2.00	0.70
2:D:82:LYS:NZ	2:D:242:GLU:OE2	2.22	0.68
1:C:17:GLN:HG2	1:C:38:TRP:HE1	1.59	0.68
2:D:139:ILE:HG23	2:D:191:LEU:HB3	1.74	0.68
2:D:226:ILE:HG22	2:D:351:THR:HB	1.77	0.67
2:D:248:ILE:HD13	2:D:380:PHE:HE1	1.60	0.67
1:A:182:CYS:HA	1:A:201:ALA:HB1	1.76	0.67
1:C:59:SER:HB3	1:C:89:GLY:HA2	1.77	0.67
2:D:153:ILE:HD13	2:D:181:MET:HE3	1.77	0.67
1:C:22:MET:HG3	2:D:144:LYS:HE3	1.77	0.66
1:C:206:ARG:HG3	3:C:502:SF4:S3	2.36	0.66
1:C:216:PHE:HB2	1:C:219:LEU:HG	1.79	0.66
1:C:234:ILE:O	1:C:238:LYS:NZ	2.21	0.65
1:A:98:PRO:HD2	1:A:101:GLU:HG3	1.77	0.64
2:D:66:SER:O	2:D:69:SER:HB3	1.97	0.64
2:B:74:LEU:HD22	2:B:96:ARG:HG2	1.79	0.64
2:D:385:MET:HG2	2:D:415:TYR:CD2	2.32	0.64
1:C:73:ARG:NH2	1:C:77:LYS:O	2.31	0.63
2:D:63:ARG:HA	2:D:160:HIS:CE1	2.33	0.63
2:D:191:LEU:HD12	2:D:191:LEU:H	1.64	0.63
1:A:29:LEU:CD1	1:A:143:LEU:HD12	2.29	0.62
2:D:119:ASP:HB3	2:D:410:MET:HE2	1.81	0.62
2:D:353:ALA:O	2:D:356:GLY:N	2.25	0.62
1:C:64:GLU:HG2	2:D:39:ILE:HD11	1.81	0.62
2:B:421:CYS:CB	4:B:501:FCO:C1	2.77	0.61
2:D:218:LYS:HE3	2:D:230:TYR:HD2	1.65	0.61
1:A:246:ARG:HH21	1:A:250:MET:HE1	1.65	0.61
2:D:14:ALA:O	2:D:413:ARG:NH1	2.32	0.61
2:D:188:ALA:HA	2:D:191:LEU:HD13	1.81	0.61
1:C:12:SER:O	2:D:420:SER:OG	2.19	0.60
2:D:120:TYR:HD2	2:D:202:LEU:HG	1.65	0.60
1:C:233:ILE:HG22	1:C:237:MET:SD	2.41	0.60
2:B:26:ILE:HG22	2:B:31:VAL:HG22	1.82	0.60
1:C:88:GLN:HG2	1:C:240:PHE:O	2.02	0.59
1:C:203:ILE:HG12	3:C:502:SF4:S2	2.42	0.59
1:C:117:LYS:HZ1	1:C:118:LYS:HB3	1.68	0.59
1:C:12:SER:O	2:D:43:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HG12	1:A:88:GLN:HG3	1.85	0.59
2:D:243:LYS:C	2:D:245:ARG:H	2.09	0.59
2:D:184:GLU:HA	2:D:187:GLU:HB2	1.85	0.58
1:C:38:TRP:CE3	1:C:41:ILE:HD13	2.38	0.58
1:A:221:LYS:HG2	1:A:224:LYS:NZ	2.17	0.58
1:C:174:ILE:HD13	1:C:196:PRO:HA	1.86	0.58
2:D:182:LYS:NZ	2:D:326:ASP:OD1	2.29	0.58
1:A:230:LYS:O	1:A:234:ILE:HG13	2.04	0.58
2:D:199:PHE:HA	2:D:202:LEU:HD13	1.85	0.58
1:C:120:GLU:HG2	1:C:121:PRO:HD2	1.84	0.58
1:C:62:THR:O	1:C:66:VAL:HG23	2.05	0.57
1:C:246:ARG:HB3	1:C:246:ARG:NH1	2.18	0.57
2:B:146:LEU:HD11	2:B:150:MET:HE2	1.87	0.57
2:D:34:VAL:HG23	2:D:386:GLU:HG2	1.87	0.57
1:A:116:PRO:HG3	2:B:257:PHE:CE1	2.40	0.57
2:B:242:GLU:OE1	2:B:242:GLU:N	2.27	0.56
1:A:164:LEU:HD11	1:A:215:TRP:CZ3	2.41	0.56
2:B:91:GLU:OE1	2:B:91:GLU:N	2.30	0.56
2:B:215:LEU:HD22	2:B:268:PHE:CE2	2.40	0.56
2:B:385:MET:O	2:B:389:VAL:HG23	2.06	0.56
2:D:295:LYS:O	2:D:295:LYS:HD3	2.05	0.56
2:D:273:ILE:HG22	2:D:306:ASN:OD1	2.06	0.56
2:D:346:PHE:HD1	2:D:363:LYS:HB2	1.71	0.56
1:C:160:TYR:HB2	1:C:164:LEU:HD22	1.86	0.56
2:B:146:LEU:CD1	2:B:150:MET:HE2	2.36	0.55
1:A:116:PRO:HG3	2:B:257:PHE:HE1	1.71	0.55
1:C:91:VAL:HB	2:D:60:ILE:HG23	1.88	0.55
2:D:115:LEU:O	2:D:413:ARG:HD2	2.07	0.55
2:D:337:ARG:HH21	2:D:339:GLU:HA	1.72	0.55
2:B:350:THR:HG22	2:B:359:VAL:HG12	1.89	0.55
2:B:388:HIS:ND1	2:B:415:TYR:OH	2.30	0.55
2:D:220:ARG:HH21	2:D:228:GLY:C	2.15	0.55
1:A:58:GLY:HA2	1:A:85:CYS:HB3	1.89	0.55
2:B:355:ARG:HB2	4:B:501:FCO:N2	2.22	0.55
1:C:239:MET:HE2	2:D:60:ILE:HD11	1.87	0.55
2:B:366:ASN:O	2:B:366:ASN:OD1	2.24	0.54
2:B:242:GLU:H	2:B:242:GLU:CD	2.12	0.54
2:B:75:THR:HG1	2:B:351:THR:HG1	1.54	0.54
2:D:294:ASN:O	2:D:298:LEU:HD12	2.07	0.54
1:A:246:ARG:HE	1:A:250:MET:HE3	1.71	0.54
1:C:174:ILE:O	1:C:178:LYS:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LYS:HG2	1:A:224:LYS:HZ1	1.72	0.54
1:C:158:ILE:N	1:C:188:ARG:HH22	2.06	0.54
2:B:75:THR:HG22	2:B:360:TYR:HB2	1.90	0.54
2:D:149:TRP:O	2:D:153:ILE:HG22	2.06	0.54
2:D:134:LYS:HD2	2:D:137:ILE:HG12	1.89	0.53
2:D:388:HIS:CD2	2:D:391:MET:HE3	2.42	0.53
1:A:29:LEU:HD13	1:A:143:LEU:CD1	2.38	0.53
1:A:12:SER:HB2	3:A:501:SF4:S1	2.49	0.53
2:B:82:LYS:HA	7:B:624:HOH:O	2.09	0.53
2:B:137:ILE:HG22	2:B:141:LEU:HD13	1.91	0.53
1:C:183:LEU:HB2	1:C:202:CYS:O	2.09	0.53
2:D:15:ARG:HD3	2:D:124:SER:O	2.09	0.53
2:D:384:MET:HE3	2:D:388:HIS:CE1	2.44	0.53
1:C:91:VAL:HG21	2:D:63:ARG:HG3	1.90	0.52
1:C:117:LYS:HZ1	1:C:118:LYS:HE2	1.74	0.52
2:D:283:LEU:HD23	2:D:288:LYS:HA	1.91	0.52
2:D:349:SER:N	2:D:360:TYR:O	2.42	0.52
1:C:117:LYS:NZ	1:C:118:LYS:HB3	2.24	0.52
2:B:10:ILE:HD11	2:B:405:LYS:HG2	1.92	0.52
1:C:232:GLU:C	1:C:233:ILE:HD13	2.35	0.52
2:D:350:THR:HG22	2:D:359:VAL:HG12	1.91	0.52
1:A:195:CYS:HB2	3:A:502:SF4:S4	2.50	0.52
1:C:254:ILE:C	1:C:256:SER:H	2.16	0.52
2:B:215:LEU:O	2:B:270:VAL:HG12	2.10	0.51
2:D:154:LEU:O	2:D:163:ASN:ND2	2.41	0.51
1:C:166:CYS:SG	1:C:171:HIS:HB2	2.50	0.51
2:D:38:ILE:HD11	2:D:382:LEU:HD22	1.92	0.51
2:D:57:ALA:HB1	2:D:61:TYR:CE2	2.45	0.51
2:D:146:LEU:O	2:D:150:MET:HG3	2.10	0.51
2:D:269:MET:HG2	2:D:274:SER:OG	2.10	0.51
2:D:299:LYS:HG3	2:D:301:THR:H	1.75	0.51
1:C:95:SER:OG	1:C:97:LYS:HG3	2.10	0.51
2:D:56:GLU:O	2:D:58:LEU:N	2.44	0.51
2:B:363:LYS:HB3	2:B:371:TYR:HB3	1.91	0.51
2:B:424:HIS:CE1	7:B:604:HOH:O	2.64	0.51
2:B:94:ALA:O	2:B:98:VAL:HG23	2.11	0.51
2:D:153:ILE:HG12	2:D:173:PRO:HG3	1.93	0.51
1:A:140[B]:LYS:NZ	1:A:190:GLY:O	2.44	0.51
1:C:2:LYS:HG2	1:C:33:ALA:C	2.36	0.50
1:C:14:TYR:O	1:C:18:LEU:HB2	2.11	0.50
2:D:106:GLU:O	2:D:110:LEU:HD23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:LEU:HD21	2:D:307:ASN:O	2.11	0.50
2:B:193:GLU:OE2	2:B:286:LYS:NZ	2.27	0.50
2:B:355:ARG:HD2	4:B:501:FCO:C2	2.42	0.50
1:C:23:MET:HB3	1:C:26:LEU:HD13	1.93	0.50
1:C:32:ASN:N	1:C:32:ASN:OD1	2.44	0.50
2:B:84:VAL:HA	2:B:343:LYS:O	2.12	0.50
1:A:174:ILE:HD11	1:A:201:ALA:HA	1.94	0.50
1:A:239:MET:CG	2:B:60:ILE:HD11	2.29	0.50
2:B:146:LEU:HG	2:B:150:MET:CE	2.42	0.50
2:B:149:TRP:CZ3	2:B:181:MET:HG3	2.47	0.50
1:C:43:ARG:NH1	2:D:406:ILE:HG22	2.14	0.50
1:C:117:LYS:NZ	1:C:118:LYS:HE2	2.26	0.50
2:D:34:VAL:HG21	2:D:390:ARG:HB2	1.93	0.50
2:D:133:TYR:O	2:D:137:ILE:HG23	2.12	0.50
2:D:73:LYS:O	2:D:77:LEU:HG	2.12	0.49
2:D:288:LYS:NZ	2:D:292:GLU:OE2	2.45	0.49
2:D:337:ARG:NH2	2:D:339:GLU:HA	2.27	0.49
1:C:26:LEU:HA	1:C:29:LEU:HG	1.94	0.49
1:C:70:LYS:O	1:C:74:GLU:HG2	2.11	0.49
2:D:146:LEU:HD21	2:D:185:LEU:HD23	1.95	0.49
2:B:38:ILE:HG22	2:B:38:ILE:O	2.11	0.49
2:B:75:THR:OG1	2:B:351:THR:OG1	2.27	0.49
1:C:246:ARG:HB3	1:C:246:ARG:HH11	1.77	0.49
2:D:114:LEU:O	2:D:126:PRO:HG3	2.12	0.49
2:D:212:ILE:HG13	2:D:384:MET:CE	2.42	0.49
2:B:175:LYS:HE3	2:B:179:GLU:OE2	2.13	0.49
1:C:215:TRP:C	1:C:216:PHE:HD1	2.20	0.49
1:C:174:ILE:HG21	1:C:199:GLY:HA2	1.95	0.49
2:B:406:ILE:O	2:B:410:MET:HG3	2.13	0.49
1:A:16:CYS:HB2	1:A:57:GLU:HG3	1.94	0.48
1:A:160:TYR:HB2	1:A:164:LEU:HD22	1.95	0.48
1:A:73:ARG:NH1	1:A:129:ASP:OD2	2.37	0.48
2:D:24:ILE:HD13	2:D:393:ALA:HB2	1.96	0.48
2:D:115:LEU:C	2:D:413:ARG:HD2	2.38	0.48
2:D:248:ILE:HD13	2:D:380:PHE:CE1	2.44	0.48
1:C:113:LYS:HB2	2:D:254:GLU:OE2	2.13	0.48
2:D:38:ILE:HG13	2:D:419:ILE:HD12	1.96	0.48
2:D:288:LYS:O	2:D:292:GLU:HG2	2.12	0.48
2:B:189:LEU:HB3	2:B:190:PRO:HD3	1.95	0.48
1:A:136:PRO:HG3	2:B:159:ILE:HB	1.95	0.48
1:A:218:SER:HB3	1:A:221:LYS:CB	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:PHE:HB2	2:B:247:TYR:CE2	2.49	0.48
2:B:196:PHE:CD2	2:B:290:LEU:HD22	2.49	0.48
1:C:69:VAL:HA	1:C:72:ILE:HD11	1.95	0.48
1:C:237:MET:HB3	1:C:241:ASN:ND2	2.29	0.48
2:D:8:ILE:HD12	2:D:404:LEU:HD23	1.95	0.48
2:D:57:ALA:HB1	2:D:61:TYR:OH	2.14	0.48
2:D:116:VAL:HG21	2:D:307:ASN:OD1	2.14	0.47
2:B:192:ALA:HB2	2:B:318:ILE:HD12	1.95	0.47
1:C:158:ILE:O	1:C:188:ARG:NH2	2.47	0.47
2:D:121:ARG:HD2	2:D:133:TYR:CZ	2.49	0.47
2:D:46:GLU:OE2	2:D:373:ASP:HA	2.14	0.47
2:D:74:LEU:HD11	2:D:96:ARG:CD	2.45	0.47
2:D:79:ALA:HB3	2:D:362:LEU:HD12	1.96	0.47
1:A:39:PHE:HE2	1:A:47:GLU:HG3	1.79	0.47
2:B:91:GLU:H	2:B:91:GLU:CD	2.19	0.47
2:B:376:THR:HB	2:B:421:CYS:HB3	1.95	0.47
1:A:185:PRO:HD3	3:A:503:SF4:S4	2.55	0.47
2:B:242:GLU:HA	2:B:348:VAL:HG11	1.97	0.47
2:B:288:LYS:O	2:B:292:GLU:HG2	2.15	0.47
1:C:144:TYR:O	1:C:148:THR:OG1	2.12	0.47
2:D:353:ALA:O	2:D:355:ARG:N	2.47	0.47
2:B:212:ILE:HD12	2:B:300:GLY:O	2.15	0.47
1:C:183:LEU:N	1:C:202:CYS:HB3	2.30	0.47
2:D:45:PHE:CE2	2:D:60:ILE:HG22	2.49	0.47
1:A:164:LEU:HD11	1:A:215:TRP:CE3	2.50	0.47
1:C:88:GLN:O	1:C:121:PRO:HD3	2.15	0.47
2:B:346:PHE:HD1	2:B:363:LYS:HB2	1.80	0.46
2:B:78:GLU:OE1	2:B:349:SER:OG	2.31	0.46
2:D:45:PHE:HE2	2:D:60:ILE:HG22	1.81	0.46
2:D:61:TYR:N	2:D:62:PRO:HD2	2.30	0.46
2:B:284:TYR:HA	2:B:288:LYS:HG3	1.97	0.46
2:D:74:LEU:HD11	2:D:96:ARG:NE	2.31	0.46
2:D:120:TYR:CD2	2:D:202:LEU:HG	2.48	0.46
1:A:98:PRO:HD2	1:A:101:GLU:CG	2.46	0.46
1:A:106:VAL:O	2:B:259:LYS:NZ	2.48	0.46
2:D:332:TRP:CD2	2:D:333:PRO:HA	2.50	0.46
2:B:332:TRP:CZ3	2:B:334:ILE:HD12	2.51	0.46
1:C:99:LEU:O	1:C:103:TRP:N	2.38	0.46
1:A:218:SER:CB	1:A:221:LYS:HB2	2.39	0.46
2:B:350:THR:HA	2:B:358:LEU:O	2.16	0.46
1:C:195:CYS:HB2	1:C:196:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:MET:HB3	1:C:241:ASN:HD22	1.81	0.46
2:D:224:TYR:HB3	2:D:316:TYR:CZ	2.51	0.45
2:D:350:THR:HA	2:D:358:LEU:O	2.16	0.45
2:B:385:MET:HE1	2:B:412:VAL:HG13	1.98	0.45
1:A:221:LYS:O	1:A:224:LYS:HG2	2.16	0.45
2:B:385:MET:HG2	2:B:415:TYR:CG	2.52	0.45
2:D:161:GLN:OE1	2:D:161:GLN:N	2.48	0.45
2:D:106:GLU:HG3	2:D:144:LYS:O	2.16	0.45
2:D:153:ILE:CG1	2:D:173:PRO:HG3	2.46	0.45
2:B:156:SER:HB3	2:B:163:ASN:HB2	1.99	0.45
2:D:192:ALA:HB1	2:D:314:ILE:HG23	1.99	0.45
1:A:50:LYS:HB2	1:A:50:LYS:HE2	1.84	0.45
2:D:19:LYS:H	2:D:40:GLU:CG	2.25	0.45
2:D:21:GLY:N	2:D:37:ASN:O	2.49	0.45
2:D:43:ARG:HB3	2:D:45:PHE:CE1	2.52	0.45
2:D:207:GLU:HB2	2:D:392:MET:SD	2.57	0.45
2:D:220:ARG:HE	2:D:228:GLY:HA2	1.81	0.45
2:D:243:LYS:C	2:D:245:ARG:N	2.75	0.45
2:D:218:LYS:O	2:D:228:GLY:HA3	2.16	0.45
1:A:18:LEU:O	1:A:22:MET:HG3	2.17	0.45
2:B:108:HIS:CE1	2:B:310:GLN:HG2	2.51	0.45
2:D:253:VAL:HG12	2:D:254:GLU:H	1.82	0.45
2:B:244:TYR:CE1	2:B:245:ARG:HG2	2.51	0.45
2:B:43:ARG:NH1	2:B:63:ARG:O	2.45	0.44
1:C:120:GLU:CG	1:C:121:PRO:HD2	2.47	0.44
2:D:150:MET:HE2	2:D:181:MET:SD	2.57	0.44
2:B:250:GLU:HA	2:B:260:HIS:O	2.17	0.44
2:B:317:PHE:HA	2:B:320:ARG:HB3	1.99	0.44
2:B:224:TYR:HB3	2:B:316:TYR:CE2	2.52	0.44
1:C:3:VAL:O	1:C:33:ALA:HB1	2.17	0.44
2:B:175:LYS:HB2	2:B:332:TRP:CE2	2.52	0.44
1:C:254:ILE:C	1:C:256:SER:N	2.76	0.44
2:D:111:HIS:HA	2:D:115:LEU:HD12	1.99	0.44
2:D:392:MET:HG3	2:D:411:VAL:HG21	2.00	0.44
2:B:175:LYS:HB2	2:B:332:TRP:CZ2	2.53	0.44
2:B:240:PRO:HG2	2:B:243:LYS:CG	2.47	0.44
1:C:245:GLU:OE1	1:C:245:GLU:N	2.48	0.44
2:D:378:THR:HA	2:D:381:ASN:HB2	1.99	0.44
2:D:276:VAL:O	2:D:280:ALA:HB2	2.18	0.44
1:A:43:ARG:HB3	2:B:124:SER:HB2	1.99	0.44
2:B:421:CYS:HB3	4:B:501:FCO:C1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:PRO:HB2	2:D:160:HIS:HA	1.99	0.44
2:B:121:ARG:HH21	2:B:136:GLU:CD	2.23	0.44
2:D:299:LYS:HD2	2:D:300:GLY:H	1.83	0.44
2:D:337:ARG:HH22	2:D:340:VAL:HG22	1.83	0.44
1:A:209:ILE:HD12	1:A:209:ILE:HA	1.73	0.43
2:B:141:LEU:O	2:B:145:ASN:HB2	2.18	0.43
1:C:73:ARG:HD2	1:C:126:ILE:HD13	2.00	0.43
1:C:233:ILE:HD13	1:C:233:ILE:N	2.31	0.43
2:B:34:VAL:HG21	2:B:389:VAL:HB	1.99	0.43
2:B:361:ALA:HB3	2:B:373:ASP:HB3	2.00	0.43
2:B:405:LYS:O	2:B:409:GLU:HG3	2.17	0.43
1:C:216:PHE:N	1:C:216:PHE:CD1	2.86	0.43
2:D:257:PHE:HB3	2:D:423:VAL:HG23	2.00	0.43
1:A:120:GLU:HG3	1:A:121:PRO:HD2	2.01	0.43
1:A:140[A]:LYS:NZ	7:A:606:HOH:O	2.50	0.43
2:D:212:ILE:HD13	2:D:301:THR:HA	2.00	0.43
2:D:226:ILE:HG23	2:D:352:GLU:H	1.82	0.43
1:A:85:CYS:HB2	7:A:610:HOH:O	2.18	0.43
1:A:117:LYS:HE2	1:A:117:LYS:HB3	1.86	0.43
1:A:140[A]:LYS:HE3	1:A:140[A]:LYS:HB3	1.84	0.43
1:A:237:MET:HE2	1:A:247:VAL:HG13	2.00	0.43
2:B:213:THR:O	2:B:268:PHE:HB2	2.18	0.43
1:C:5:ILE:HB	1:C:34:GLU:O	2.19	0.43
2:D:332:TRP:CG	2:D:333:PRO:HA	2.53	0.43
1:A:4:ARG:NH1	1:A:49:GLU:OE2	2.52	0.43
2:D:106:GLU:HG2	2:D:110:LEU:CD2	2.49	0.43
2:D:272:ALA:HA	2:D:275:ARG:NH1	2.33	0.43
2:D:150:MET:HE2	2:D:181:MET:CG	2.49	0.43
2:D:311:ALA:O	2:D:314:ILE:HG22	2.19	0.43
2:B:376:THR:HB	4:B:501:FCO:N1	2.34	0.43
1:C:216:PHE:O	1:C:217:ASP:C	2.61	0.43
2:D:111:HIS:CE1	2:D:416:ASP:HB2	2.54	0.43
2:D:227:TYR:HA	2:D:351:THR:HG22	2.00	0.43
2:D:378:THR:HG21	2:D:418:CYS:C	2.44	0.43
1:A:136:PRO:HB3	3:A:501:SF4:S3	2.59	0.42
2:D:353:ALA:N	2:D:356:GLY:O	2.51	0.42
2:B:86:PHE:CD1	2:B:340:VAL:HG22	2.54	0.42
2:D:199:PHE:CD2	2:D:202:LEU:HD22	2.54	0.42
2:B:87:VAL:HG12	2:B:88:PRO:O	2.20	0.42
1:C:5:ILE:HG12	1:C:53:ILE:HB	2.00	0.42
1:A:2:LYS:NZ	1:A:31:PRO:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:LEU:CD1	1:C:26:LEU:HD21	2.49	0.42
2:D:353:ALA:C	2:D:355:ARG:N	2.78	0.42
2:D:385:MET:HE2	2:D:385:MET:HB3	1.54	0.42
2:D:145:ASN:HA	2:D:148:THR:HG22	2.00	0.42
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.69	0.42
1:A:40:MET:O	2:B:15:ARG:HA	2.19	0.42
2:D:355:ARG:HB2	2:D:377:PRO:HG2	2.02	0.42
1:A:99:LEU:HD22	1:A:99:LEU:HA	1.83	0.42
1:C:25:GLU:HG2	1:C:28:GLN:HE22	1.84	0.42
1:C:134:GLY:HA2	1:C:206:ARG:HG2	2.01	0.42
2:B:377:PRO:CD	4:B:501:FCO:N1	2.68	0.42
1:C:175:LEU:HG	1:C:181:PRO:CA	2.47	0.42
2:D:92:ILE:O	2:D:96:ARG:HG3	2.20	0.42
2:D:177:VAL:HG13	2:D:180:LYS:NZ	2.35	0.42
2:B:424:HIS:N	7:B:609:HOH:O	2.53	0.41
2:D:68:CYS:O	2:D:72:HIS:ND1	2.32	0.41
2:B:276:VAL:O	2:B:280:ALA:HB2	2.20	0.41
1:C:61:SER:O	1:C:117:LYS:N	2.54	0.41
1:C:167:ARG:O	1:C:167:ARG:NE	2.53	0.41
2:D:97:GLU:OE1	2:D:226:ILE:HB	2.20	0.41
1:A:224:LYS:HG2	1:A:225:GLU:N	2.34	0.41
2:B:77:LEU:HD23	2:B:77:LEU:HA	1.94	0.41
1:C:69:VAL:HA	1:C:72:ILE:CD1	2.50	0.41
1:C:175:LEU:HD23	1:C:175:LEU:C	2.46	0.41
2:D:74:LEU:HD11	2:D:96:ARG:HD3	2.02	0.41
2:D:217:VAL:HB	2:D:352:GLU:OE2	2.21	0.41
2:B:17:GLU:HB3	2:B:418:CYS:HA	2.03	0.41
2:B:229:ASP:C	2:B:241:SER:HG	2.28	0.41
1:C:167:ARG:O	1:C:167:ARG:CZ	2.69	0.41
2:D:60:ILE:N	2:D:60:ILE:HD12	2.35	0.41
2:D:110:LEU:O	2:D:114:LEU:HB2	2.20	0.41
2:B:424:HIS:NE2	7:B:604:HOH:O	2.37	0.41
1:C:138:GLU:HG3	1:C:190:GLY:O	2.21	0.41
1:C:161:PRO:O	1:C:189:ALA:HB2	2.21	0.41
2:D:217:VAL:HG23	2:D:357:ILE:HG12	2.03	0.41
1:A:66:VAL:O	1:A:70:LYS:HG3	2.21	0.41
1:C:162:VAL:HG23	1:C:187:THR:O	2.20	0.41
2:D:56:GLU:C	2:D:58:LEU:N	2.79	0.41
2:D:378:THR:HG21	2:D:418:CYS:O	2.21	0.41
1:A:18:LEU:HD11	2:B:110:LEU:HD11	2.03	0.40
2:B:144:LYS:NZ	2:B:145:ASN:OD1	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:VAL:HG21	2:D:351:THR:O	2.20	0.40
2:B:49:THR:HB	2:B:57:ALA:HB1	2.04	0.40
2:D:409:GLU:O	2:D:413:ARG:N	2.48	0.40
1:A:166:CYS:SG	1:A:171:HIS:HB2	2.62	0.40
1:C:78:ILE:HG21	1:C:149:PHE:CZ	2.57	0.40
1:C:163:CYS:SG	1:C:185:PRO:HD3	2.61	0.40
2:D:205:TYR:CD1	2:D:205:TYR:N	2.87	0.40
2:D:355:ARG:CB	2:D:377:PRO:HG2	2.50	0.40
2:D:419:ILE:HA	2:D:422:SER:CB	2.51	0.40
1:A:22:MET:HE1	2:B:106:GLU:OE2	2.22	0.40
2:B:44:PHE:O	2:B:48:ILE:HG12	2.21	0.40
2:D:74:LEU:HD13	2:D:77:LEU:HD12	2.03	0.40
2:D:397:TYR:HA	2:D:404:LEU:HD22	2.02	0.40
2:D:304:PHE:CE1	2:D:411:VAL:HG22	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	255/256 (100%)	245 (96%)	10 (4%)	0	100	100
1	C	250/256 (98%)	214 (86%)	27 (11%)	9 (4%)	3	4
2	B	418/419 (100%)	392 (94%)	21 (5%)	5 (1%)	11	24
2	D	417/419 (100%)	387 (93%)	24 (6%)	6 (1%)	9	19
All	All	1340/1350 (99%)	1238 (92%)	82 (6%)	20 (2%)	8	18

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	181	PRO

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Mol	Chain	Res	Type
1	C	182	CYS
1	C	234	ILE
2	D	56	GLU
2	D	57	ALA
2	B	156	SER
1	C	38	TRP
1	C	252	ALA
2	D	244	TYR
2	B	87	VAL
2	B	342	ILE
1	C	27	LEU
1	C	217	ASP
1	C	253	LYS
2	D	53	LYS
1	C	94	TRP
2	D	224	TYR
2	B	157	ARG
2	B	399	ASP
2	D	354	PRO

### 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	216/215 (100%)	205 (95%)	11 (5%)	20	42
1	C	213/215 (99%)	198 (93%)	15 (7%)	12	27
2	B	351/350 (100%)	341 (97%)	10 (3%)	38	65
2	D	350/350 (100%)	331 (95%)	19 (5%)	18	39
All	All	1130/1130 (100%)	1075 (95%)	55 (5%)	21	43

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	60	VAL

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Mol	Chain	Res	Type
1	A	64	GLU
1	A	88	GLN
1	A	93	SER
1	A	95	SER
1	A	109	ASP
1	A	200	VAL
1	A	202	CYS
1	A	235	GLU
1	A	247	VAL
2	B	34	VAL
2	B	69	SER
2	B	73	LYS
2	B	110	LEU
2	B	186	ARG
2	B	195	THR
2	B	237	GLU
2	B	253	VAL
2	B	288	LYS
2	B	348	VAL
1	C	32	ASN
1	C	41	ILE
1	C	59	SER
1	C	63	GLU
1	C	72	ILE
1	C	99	LEU
1	C	114	PHE
1	C	157	ASP
1	C	182	CYS
1	C	224	LYS
1	C	225	GLU
1	C	235	GLU
1	C	236	ARG
1	C	247	VAL
1	C	254	ILE
2	D	13	ILE
2	D	28	ASP
2	D	69	SER
2	D	74	LEU
2	D	99	LEU
2	D	119	ASP
2	D	127	LEU
2	D	137	ILE

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Mol	Chain	Res	Type
2	D	142	LYS
2	D	146	LEU
2	D	153	ILE
2	D	176	SER
2	D	227	TYR
2	D	248	ILE
2	D	252	VAL
2	D	322	ILE
2	D	331	LYS
2	D	341	GLU
2	D	421	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
2	B	294	ASN
2	B	366	ASN
1	C	28	GLN
2	D	160	HIS
2	D	279	ASN
2	D	366	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

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	FCO	B	501	2	0,6,6	-	-	-		
3	SF4	C	504	-	0,12,12	-	-	-		
3	SF4	C	502	1	0,12,12	-	-	-		
3	SF4	A	501	1	0,12,12	-	-	-		
3	SF4	C	505	-	0,12,12	-	-	-		
3	SF4	A	503	1	0,12,12	-	-	-		
3	SF4	A	502	1	0,12,12	-	-	-		
3	SF4	C	503	1	0,12,12	-	-	-		
3	SF4	C	501	1	0,12,12	-	-	-		

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
3	SF4	C	504	-	-	-	0/6/5/5
3	SF4	C	502	1	-	-	0/6/5/5
3	SF4	A	501	1	-	-	0/6/5/5
3	SF4	C	505	-	-	-	0/6/5/5
3	SF4	A	503	1	-	-	0/6/5/5
3	SF4	A	502	1	-	-	0/6/5/5
3	SF4	C	503	1	-	-	0/6/5/5
3	SF4	C	501	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	FCO	8	0
3	C	502	SF4	2	0
3	A	501	SF4	2	0
3	A	503	SF4	1	0
3	A	502	SF4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	256/256 (100%)	0.19	2 (0%) 82 79	19, 41, 60, 75	1 (0%)
1	C	253/256 (98%)	3.77	198 (78%) 0 0	6, 36, 51, 69	250 (98%)
2	B	419/419 (100%)	0.18	9 (2%) 63 58	22, 36, 56, 83	1 (0%)
2	D	419/419 (100%)	3.45	330 (78%) 0 0	8, 38, 54, 70	409 (97%)
All	All	1347/1350 (99%)	1.87	539 (40%) 1 1	6, 37, 56, 83	661 (49%)

All (539) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	13	ILE	13.3
1	C	255	PHE	12.8
2	D	264	LYS	12.7
1	C	226	ALA	12.0
2	D	51	GLY	11.8
1	C	223	PHE	11.7
1	C	247	VAL	11.4
1	C	221	LYS	11.3
1	C	231	GLU	11.0
2	D	359	VAL	10.8
1	C	252	ALA	10.5
1	C	187	THR	10.3
1	C	87	VAL	10.3
1	C	230	LYS	10.3
2	D	416	ASP	9.6
2	D	130	VAL	9.4
2	D	52	LYS	9.4
2	D	424	HIS	9.3
2	D	270	VAL	9.2
2	D	386	GLU	9.1
2	D	64	ILE	9.0

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Mol	Chain	Res	Type	RSRZ
1	C	228	MET	9.0
2	D	289	GLU	8.5
1	C	222	VAL	8.5
1	C	236	ARG	8.3
1	C	184	GLY	8.3
2	D	300	GLY	8.2
1	C	225	GLU	8.2
2	D	367	GLY	8.1
2	D	321	ALA	8.1
1	C	182	CYS	8.0
2	D	365	GLU	7.9
1	C	86	ALA	7.9
1	C	110	ALA	7.9
2	D	31	VAL	7.9
1	C	106	VAL	7.7
1	C	205	CYS	7.7
1	C	64	GLU	7.6
2	D	357	ILE	7.4
1	C	22	MET	7.4
1	C	211	TYR	7.4
1	C	254	ILE	7.3
1	C	109	ASP	7.3
2	D	267	PRO	7.2
1	C	35	ILE	7.2
1	C	248	GLU	7.2
2	D	168	GLY	7.2
1	C	235	GLU	7.1
2	D	20	GLY	7.1
1	C	203	ILE	7.1
2	D	26	ILE	7.0
1	C	21	ALA	6.9
2	D	103	ASP	6.9
2	D	133	TYR	6.9
1	C	240	PHE	6.8
2	D	268	PHE	6.8
1	C	251	VAL	6.7
2	D	134	LYS	6.6
2	D	361	ALA	6.6
2	D	418	CYS	6.5
1	C	27	LEU	6.4
1	C	170	GLY	6.3
2	D	250	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
2	D	391	MET	6.2
2	D	25	ILE	6.1
1	C	219	LEU	6.1
2	D	336	PRO	6.1
2	D	193	GLU	6.1
1	C	114	PHE	6.1
2	D	251	PHE	6.1
2	D	366	ASN	6.0
1	C	229	THR	6.0
2	D	28	ASP	6.0
2	D	65	CYS	5.9
1	C	11	THR	5.9
2	D	45	PHE	5.9
2	D	394	GLU	5.9
2	D	397	TYR	5.9
1	C	190	GLY	5.9
2	D	141	LEU	5.9
2	D	10	ILE	5.8
1	C	189	ALA	5.8
2	D	127	LEU	5.8
1	C	24	ASP	5.8
2	D	41	GLY	5.8
1	C	200	VAL	5.7
2	D	122	GLY	5.7
2	D	57	ALA	5.7
1	C	107	TYR	5.7
2	D	50	ILE	5.7
2	D	305	ALA	5.6
2	D	211	PRO	5.6
2	D	30	GLY	5.6
2	D	379	ALA	5.6
1	C	94	TRP	5.6
2	D	135	ARG	5.5
2	D	398	ASN	5.5
2	D	29	ASP	5.5
2	D	139	ILE	5.5
1	C	93	SER	5.5
2	D	138	GLU	5.5
1	C	139	LYS	5.4
2	D	8	ILE	5.4
2	D	244	TYR	5.4
2	D	406	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
2	D	54	LEU	5.4
1	C	91	VAL	5.4
2	D	387	GLU	5.3
1	C	29	LEU	5.3
1	C	166	CYS	5.3
2	D	317	PHE	5.2
2	D	44	PHE	5.2
1	C	169	ASN	5.2
2	D	189	LEU	5.2
1	C	249	LYS	5.2
1	C	39	PHE	5.2
1	C	81	ALA	5.1
2	D	11	ASP	5.1
1	C	253	LYS	5.1
2	D	248	ILE	5.1
2	D	55	GLU	5.0
2	D	83	ALA	5.0
2	D	376	THR	5.0
1	C	58	GLY	4.9
2	D	167	GLY	4.9
1	C	40	MET	4.9
1	C	131	ASN	4.9
2	D	208	VAL	4.9
1	C	143	LEU	4.9
2	D	349	SER	4.9
2	D	194	TYR	4.9
2	D	421	CYS	4.8
2	D	417	PRO	4.8
2	D	210	GLY	4.8
1	C	201	ALA	4.8
1	C	7	PHE	4.8
2	D	137	ILE	4.8
2	D	375	ILE	4.8
2	D	53	LYS	4.8
2	D	58	LEU	4.8
2	D	297	LEU	4.7
2	D	62	PRO	4.7
2	D	401	PRO	4.7
2	D	155	GLY	4.7
2	D	279	ASN	4.7
1	C	84	ALA	4.7
1	C	49	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	358	LEU	4.7
2	D	123	TYR	4.7
1	C	68	LEU	4.7
2	D	404	LEU	4.7
1	C	174	ILE	4.6
2	D	183	ALA	4.6
2	D	256	SER	4.6
2	D	415	TYR	4.6
2	D	263	TYR	4.6
2	D	117	LEU	4.6
2	D	129	MET	4.6
2	D	22	VAL	4.6
1	C	99	LEU	4.5
2	D	227	TYR	4.5
1	C	75	ASN	4.5
1	C	113	LYS	4.5
2	D	109	ALA	4.5
2	D	73	LYS	4.5
2	D	393	ALA	4.5
2	D	316	TYR	4.4
1	C	112	VAL	4.4
1	C	173	CYS	4.4
2	D	230	TYR	4.4
2	D	247	TYR	4.4
1	C	234	ILE	4.4
2	D	143	LEU	4.4
2	D	181	MET	4.4
1	C	32	ASN	4.4
2	D	261	SER	4.4
2	D	414	ALA	4.4
2	D	284	TYR	4.3
2	D	371	TYR	4.3
2	D	381	ASN	4.3
2	D	249	LYS	4.3
2	D	271	GLY	4.3
1	C	101	GLU	4.3
1	C	19	GLN	4.3
1	C	194	ARG	4.3
2	D	32	LYS	4.3
1	C	10	LEU	4.3
1	C	3	VAL	4.3
2	D	101	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	306	ASN	4.2
2	D	7	PRO	4.2
2	D	303	PRO	4.2
2	D	17	GLU	4.2
1	C	210	GLY	4.2
1	C	208	ALA	4.2
2	D	128	LYS	4.2
2	D	40	GLU	4.2
1	C	26	LEU	4.2
2	D	147	GLY	4.2
1	C	172	PRO	4.2
2	D	36	LEU	4.1
2	D	287	ALA	4.1
1	C	185	PRO	4.1
2	D	282	LEU	4.1
1	C	239	MET	4.1
1	C	180	GLU	4.1
2	D	33	GLU	4.1
2	D	280	ALA	4.1
1	C	28	GLN	4.1
2	D	71	ALA	4.0
2	D	277	ILE	4.0
2	D	84	VAL	4.0
2	D	21	GLY	4.0
1	C	98	PRO	4.0
1	C	137	PRO	4.0
2	D	42	PRO	4.0
2	D	222	ASP	4.0
2	D	131	ASN	4.0
2	D	177	VAL	4.0
2	D	373	ASP	4.0
1	C	224	LYS	4.0
2	D	113	TYR	4.0
1	C	181	PRO	4.0
2	D	74	LEU	4.0
2	D	382	LEU	4.0
1	C	45	SER	3.9
2	D	146	LEU	3.9
1	C	204	GLY	3.9
1	C	177	GLU	3.9
2	D	120	TYR	3.9
2	D	231	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	257	PHE	3.9
2	D	302	ASN	3.9
1	C	34	GLU	3.8
2	B	222	ASP	3.8
1	C	183	LEU	3.8
1	C	175	LEU	3.8
2	D	360	TYR	3.8
1	C	215	TRP	3.8
1	C	157	ASP	3.8
1	C	176	LEU	3.8
2	D	156	SER	3.8
1	C	83	GLY	3.8
2	D	116	VAL	3.8
2	D	142	LYS	3.8
2	D	368	ARG	3.8
2	D	314	ILE	3.8
2	D	14	ALA	3.7
2	D	329	LEU	3.7
2	D	362	LEU	3.7
1	C	186	VAL	3.7
1	C	115	GLN	3.7
1	C	199	GLY	3.7
1	C	168	LEU	3.7
2	D	276	VAL	3.7
2	D	157	ARG	3.7
2	D	241	SER	3.7
2	D	262	HIS	3.7
1	C	160	TYR	3.7
1	C	48	ASP	3.7
2	D	419	ILE	3.7
2	D	204	GLN	3.6
1	C	15	GLY	3.6
1	C	147	GLY	3.6
1	C	14	TYR	3.6
2	D	342	ILE	3.6
2	D	374	ILE	3.6
1	C	133	TYR	3.6
2	D	380	PHE	3.6
1	C	37	CYS	3.6
1	C	149	PHE	3.6
2	D	304	PHE	3.6
2	B	281	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	327	GLU	3.5
2	D	16	VAL	3.5
2	D	213	THR	3.5
1	C	246	ARG	3.5
1	C	66	VAL	3.5
1	C	162	VAL	3.5
2	D	105	ILE	3.5
2	D	144	LYS	3.5
2	D	212	ILE	3.5
1	C	119	ALA	3.5
1	C	123	SER	3.5
1	C	218	SER	3.5
2	D	423	VAL	3.5
2	D	334	ILE	3.5
2	D	239	PHE	3.5
2	D	112	LEU	3.5
1	C	141	ASP	3.5
1	C	232	GLU	3.4
1	C	238	LYS	3.4
2	D	315	VAL	3.4
1	C	89	GLY	3.4
2	D	326	ASP	3.4
2	D	392	MET	3.4
2	D	372	ALA	3.4
2	D	12	HIS	3.4
2	D	27	GLY	3.4
2	D	191	LEU	3.4
2	D	96	ARG	3.4
2	D	405	LYS	3.4
2	D	340	VAL	3.3
2	D	348	VAL	3.3
1	C	250	MET	3.3
2	D	228	GLY	3.3
1	C	95	SER	3.3
1	C	120	GLU	3.3
2	D	81	GLU	3.3
1	C	88	GLN	3.3
2	D	166	LEU	3.3
2	D	209	GLU	3.3
2	D	216	ALA	3.3
2	D	384	MET	3.3
2	D	152	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	91	GLU	3.3
2	D	132	GLU	3.3
2	D	407	LEU	3.3
1	C	57	GLU	3.2
2	D	176	SER	3.2
2	D	215	LEU	3.2
2	D	245	ARG	3.2
1	C	33	ALA	3.2
1	C	60	VAL	3.2
2	D	333	PRO	3.2
2	D	47	ALA	3.2
2	D	269	MET	3.2
2	D	214	HIS	3.2
2	D	311	ALA	3.2
1	C	206	ARG	3.2
2	D	413	ARG	3.2
1	C	214	ALA	3.1
2	D	309	ALA	3.1
1	C	122	VAL	3.1
2	D	266	ARG	3.1
1	C	191	CYS	3.1
2	D	385	MET	3.1
2	D	106	GLU	3.1
1	C	111	LYS	3.1
1	C	46	ILE	3.1
2	D	159	ILE	3.1
2	D	158	ALA	3.1
2	D	411	VAL	3.1
2	D	301	THR	3.1
2	D	59	ALA	3.1
2	D	161	GLN	3.1
1	C	179	GLY	3.1
1	C	8	TYR	3.1
1	C	165	GLU	3.1
1	C	51	VAL	3.1
1	C	161	PRO	3.1
2	D	136	GLU	3.0
2	D	283	LEU	3.0
2	D	252	VAL	3.0
2	D	253	VAL	3.0
2	D	320	ARG	3.0
2	D	255	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	170	GLY	3.0
1	C	156	GLU	3.0
1	C	72	ILE	3.0
1	C	126	ILE	3.0
1	C	163	CYS	3.0
1	C	69	VAL	3.0
2	D	233	ALA	3.0
1	C	108	GLY	3.0
2	D	97	GLU	2.9
2	D	115	LEU	2.9
1	C	243	HIS	2.9
2	D	86	PHE	2.9
1	C	227	GLY	2.9
2	D	162	GLU	2.9
1	C	103	TRP	2.9
2	D	275	ARG	2.9
1	C	130	TYR	2.9
1	C	65	GLU	2.9
2	D	63	ARG	2.9
2	D	346	PHE	2.9
1	C	100	GLU	2.8
2	D	46	GLU	2.8
2	D	322	ILE	2.8
2	D	61	TYR	2.8
1	C	20	LEU	2.8
2	D	288	LYS	2.8
2	D	388	HIS	2.8
2	D	354	PRO	2.8
1	C	197	GLY	2.8
2	D	24	ILE	2.8
2	D	364	VAL	2.8
2	D	224	TYR	2.8
1	C	4	ARG	2.8
2	D	226	ILE	2.8
1	C	245	GLU	2.8
1	C	213	VAL	2.8
1	C	154	TRP	2.8
2	D	195	THR	2.8
2	D	121	ARG	2.8
1	C	63	GLU	2.7
2	D	369	VAL	2.7
2	D	389	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	79	ALA	2.7
2	D	258	ALA	2.7
2	D	19	LYS	2.7
2	D	352	GLU	2.7
2	D	87	VAL	2.7
1	C	153	SER	2.7
2	D	95	LEU	2.7
2	B	221	GLY	2.7
2	D	355	ARG	2.7
1	C	144	TYR	2.7
1	C	217	ASP	2.7
1	C	56	ILE	2.7
2	D	92	ILE	2.7
2	D	259	LYS	2.7
1	C	193	ALA	2.7
2	D	114	LEU	2.7
2	D	125	SER	2.7
2	D	100	TYR	2.6
1	C	38	TRP	2.6
2	D	356	GLY	2.6
2	D	174	GLU	2.6
2	D	56	GLU	2.6
2	D	90	GLU	2.6
2	D	93	GLN	2.6
2	D	219	PRO	2.6
1	C	117	LYS	2.6
2	D	23	GLU	2.6
2	D	344	ASP	2.6
2	D	99	LEU	2.6
2	D	185	LEU	2.6
2	D	307	ASN	2.6
2	D	118	PRO	2.6
2	D	85	GLY	2.6
2	D	298	LEU	2.5
2	D	229	ASP	2.5
1	C	79	VAL	2.5
1	C	241	ASN	2.5
2	D	278	ASN	2.5
2	D	310	GLN	2.5
2	D	408	ALA	2.5
2	B	46	GLU	2.5
1	C	237	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	104	LYS	2.5
2	D	232	LYS	2.5
1	C	188	ARG	2.5
2	D	390	ARG	2.5
2	D	67	PHE	2.5
2	D	175	LYS	2.5
2	D	292	GLU	2.4
2	D	332	TRP	2.4
1	C	198	PHE	2.4
2	D	205	TYR	2.4
1	C	134	GLY	2.4
1	C	242	GLY	2.4
2	D	9	THR	2.4
2	D	148	THR	2.4
2	D	187	GLU	2.4
1	C	17	GLN	2.4
2	D	66	SER	2.4
2	D	383	ALA	2.4
1	C	140	LYS	2.4
2	D	190	PRO	2.4
1	C	82	VAL	2.4
2	D	199	PHE	2.4
2	D	18	GLY	2.4
2	B	246	ASP	2.4
2	D	396	HIS	2.3
2	D	149	TRP	2.3
2	D	274	SER	2.3
2	D	330	ALA	2.3
2	D	221	GLY	2.3
1	C	125	TYR	2.3
1	C	67	GLU	2.3
1	C	118	LYS	2.3
1	C	196	PRO	2.3
1	C	171	HIS	2.3
1	C	80	VAL	2.3
2	D	34	VAL	2.3
2	D	169	PHE	2.3
1	C	62	THR	2.3
2	B	97	GLU	2.3
1	C	142	PHE	2.3
1	C	145	ALA	2.3
2	D	377	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	6	LEU	2.3
2	D	395	LYS	2.2
2	D	422	SER	2.3
2	D	350	THR	2.2
1	C	202	CYS	2.2
2	D	108	HIS	2.2
2	D	318	ILE	2.2
2	D	140	ALA	2.2
1	A	94	TRP	2.2
1	C	256	SER	2.2
2	D	124	SER	2.2
2	D	402	GLU	2.2
2	D	49	THR	2.2
1	C	244	ASP	2.2
2	D	104	MET	2.2
2	D	412	VAL	2.2
2	D	171	LYS	2.2
1	C	61	SER	2.2
2	D	111	HIS	2.2
1	C	41	ILE	2.2
1	C	195	CYS	2.2
1	C	150	LEU	2.2
1	C	164	LEU	2.2
2	D	236	GLY	2.2
2	D	378	THR	2.1
2	D	145	ASN	2.1
1	C	44	ASP	2.1
2	D	173	PRO	2.1
2	D	182	LYS	2.1
2	D	325	LEU	2.1
2	D	223	ALA	2.1
1	C	1	GLY	2.1
1	C	138	GLU	2.1
2	B	394	GLU	2.1
2	D	242	GLU	2.1
1	C	59	SER	2.1
2	D	206	SER	2.1
2	D	331	LYS	2.1
2	D	399	ASP	2.1
2	D	200	ALA	2.1
2	D	328	ALA	2.1
2	D	260	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	75	THR	2.1
2	D	154	LEU	2.1
1	A	109	ASP	2.1
2	D	88	PRO	2.0
2	D	153	ILE	2.0
2	D	217	VAL	2.0
1	C	167	ARG	2.0
2	D	400	ASP	2.0
2	D	160	HIS	2.0
2	D	351	THR	2.0
1	C	43	ARG	2.0
2	D	234	SER	2.0
2	B	230	TYR	2.0
2	D	246	ASP	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 oligosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	SF4	C	504	8/8	0.57	0.20	107,117,129,141	8
3	SF4	C	505	8/8	0.63	0.20	54,78,100,103	8
3	SF4	C	502	8/8	0.77	0.17	49,64,76,84	8
3	SF4	C	503	8/8	0.86	0.11	59,74,85,88	8
3	SF4	C	501	8/8	0.90	0.12	49,58,73,75	8
6	CL	B	503	1/1	0.90	0.11	66,66,66,66	0
5	NI	B	502	1/1	0.92	0.06	52,52,52,52	0
4	FCO	B	501	7/7	0.95	0.18	8,9,11,13	0
5	NI	D	501	1/1	0.97	0.06	61,61,61,61	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SF4	A	501	8/8	0.98	0.05	22,23,25,26	0
3	SF4	A	502	8/8	0.98	0.04	20,24,27,27	0
3	SF4	A	503	8/8	0.98	0.04	22,27,29,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.