



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 05:01 AM EDT

PDB ID : 6DQG  
Title : Human glutamate dehydrogenase, H454Y mutant  
Authors : Smith, T.J.  
Deposited on : 2018-06-10  
Resolution : 2.70 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 : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

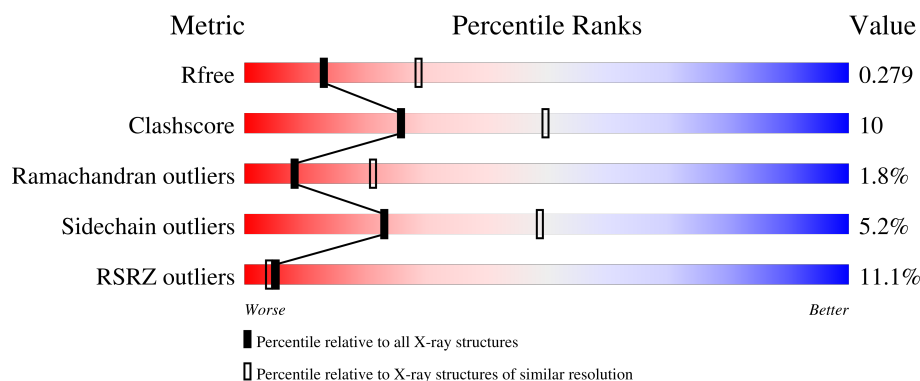
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	496	<div> <div>13%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	B	496	<div> <div>8%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
1	C	496	<div> <div>19%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
1	D	496	<div> <div>9%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
1	E	496	<div> <div>4%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	496	

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
2	PO4	A	1001	-	-	X	-
2	PO4	D	603	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23591 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.

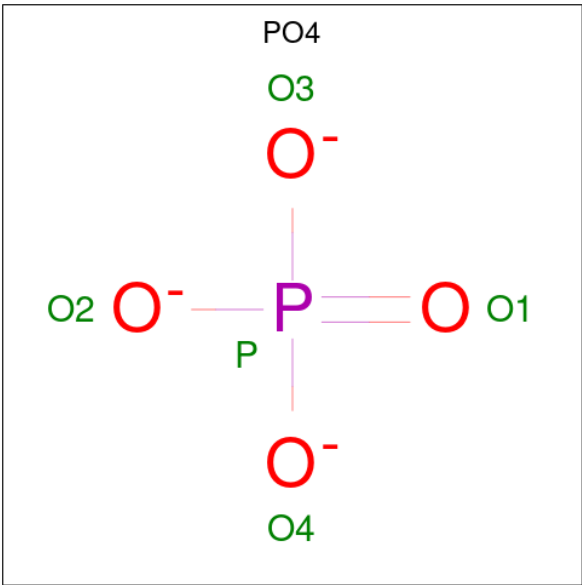
- Molecule 1 is a protein called Glutamate dehydrogenase 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3876	2453	677	727	19			
1	B	496	Total	C	N	O	S	0	0	0
			3876	2453	677	727	19			
1	C	496	Total	C	N	O	S	0	0	0
			3876	2453	677	727	19			
1	D	496	Total	C	N	O	S	0	0	0
			3876	2453	677	727	19			
1	E	496	Total	C	N	O	S	0	0	0
			3876	2453	677	727	19			
1	F	496	Total	C	N	O	S	0	0	0
			3876	2453	677	727	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	TYR	HIS	engineered mutation	UNP P00367
B	454	TYR	HIS	engineered mutation	UNP P00367
C	454	TYR	HIS	engineered mutation	UNP P00367
D	454	TYR	HIS	engineered mutation	UNP P00367
E	454	TYR	HIS	engineered mutation	UNP P00367
F	454	TYR	HIS	engineered mutation	UNP P00367

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	P	0	0
			5	4	1		

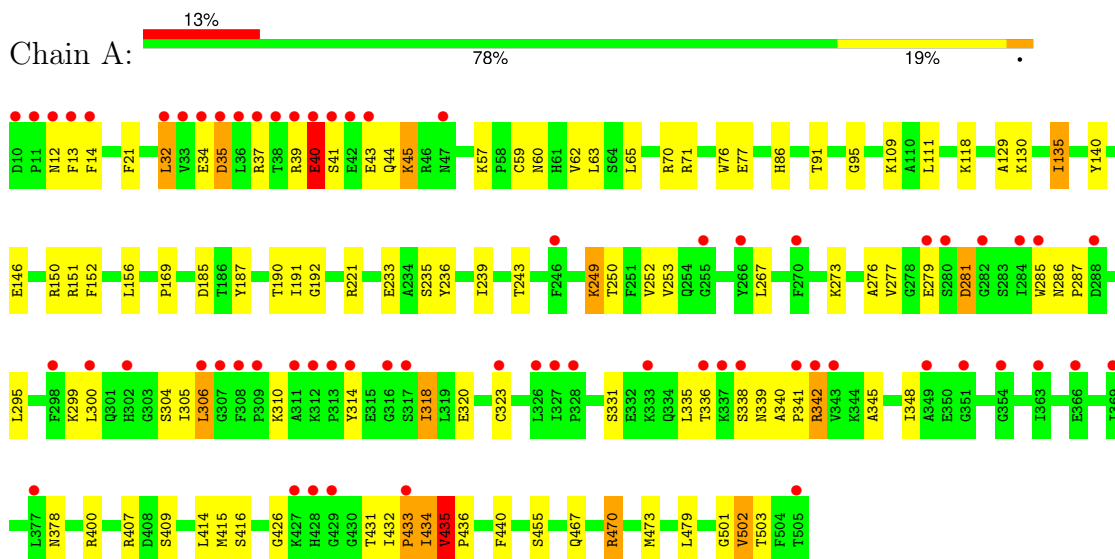
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	51	Total	O	0	0
			51	51		
3	C	46	Total	O	0	0
			46	46		
3	D	49	Total	O	0	0
			49	49		
3	E	47	Total	O	0	0
			47	47		
3	F	36	Total	O	0	0
			36	36		

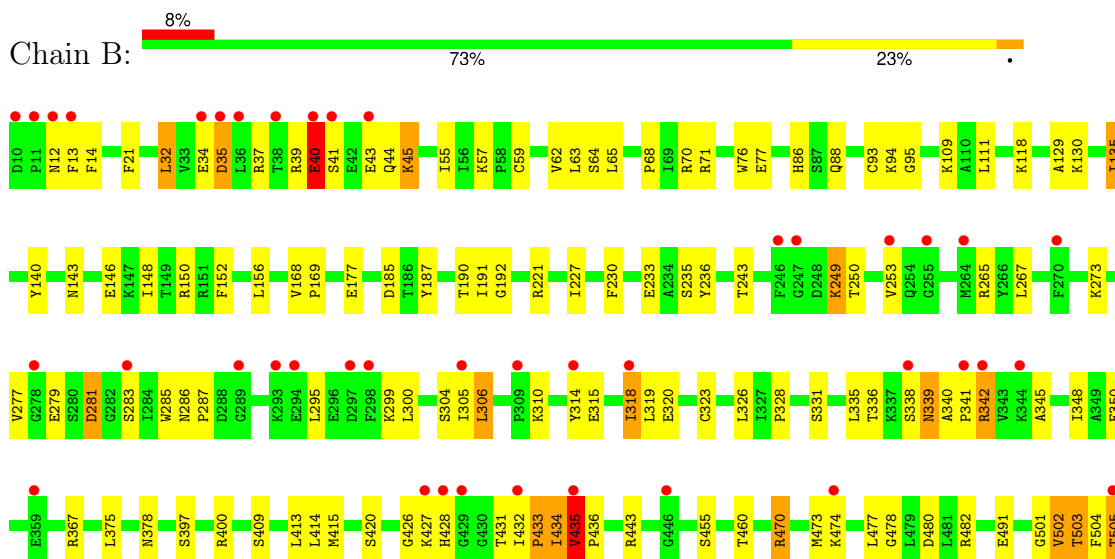
### 3 Residue-property plots

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: Glutamate dehydrogenase 1, mitochondrial



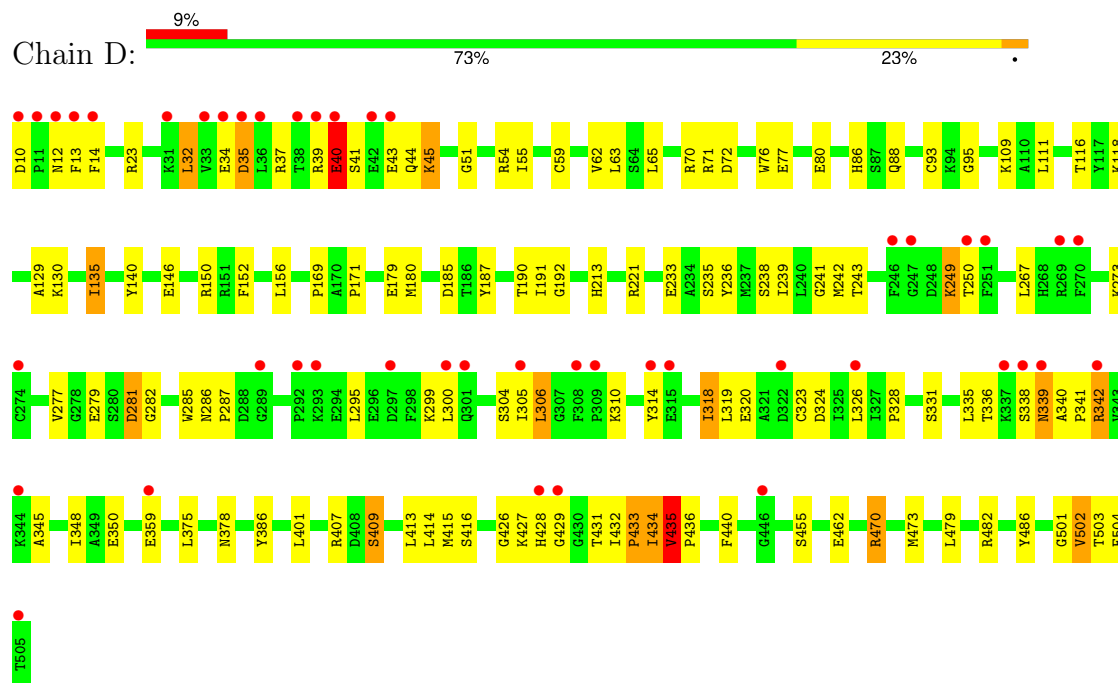
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



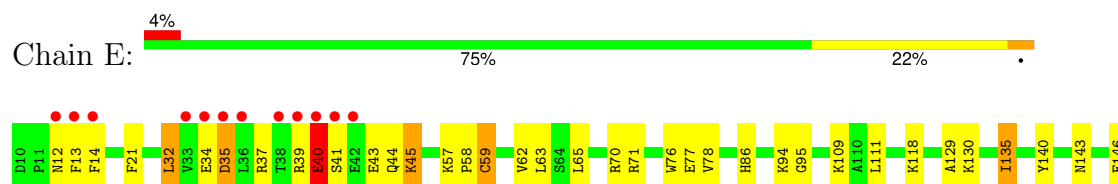
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

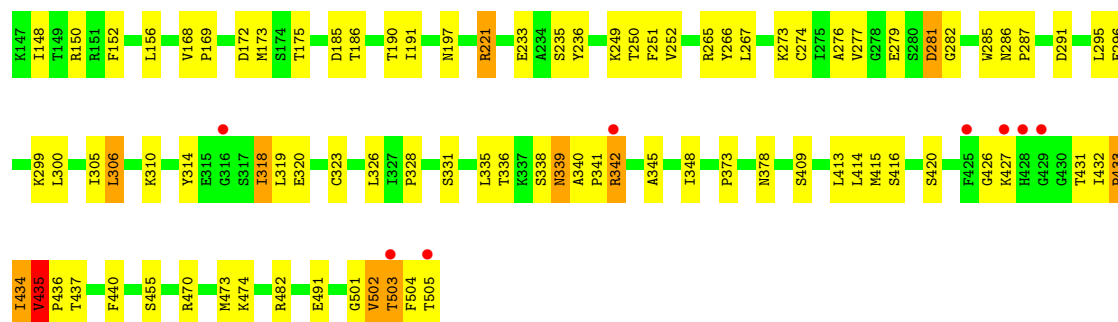


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

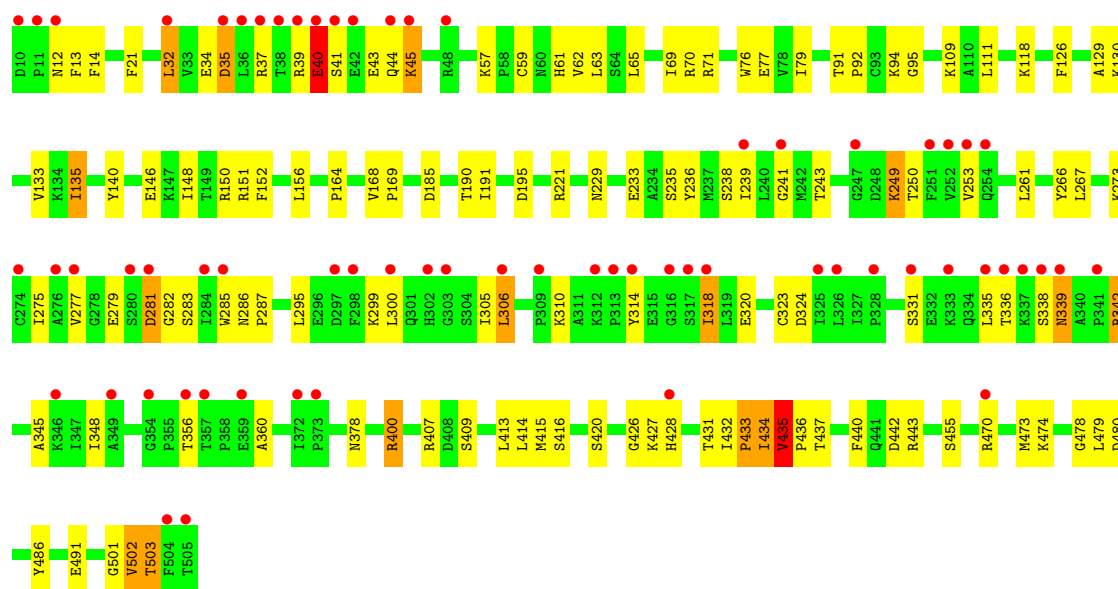
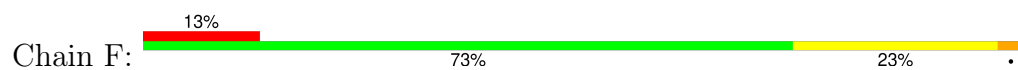


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial





● Molecule 1: Glutamate dehydrogenase 1, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.80Å 98.38Å 124.30Å 85.94° 69.35° 61.00°	Depositor
Resolution (Å)	29.77 – 2.70 29.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.9 (29.77-2.70) 88.9 (29.77-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.63 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.241 , 0.279 0.243 , 0.279	Depositor DCC
$R_{free}$ test set	4609 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for h,h-k,h-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23591	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: PO4

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	0.41	0/3960	0.69	3/5343 (0.1%)
1	B	0.44	0/3960	0.69	4/5343 (0.1%)
1	C	0.47	0/3960	0.83	6/5343 (0.1%)
1	D	0.43	0/3960	0.59	2/5343 (0.0%)
1	E	0.44	1/3960 (0.0%)	0.57	1/5343 (0.0%)
1	F	0.43	0/3960	0.58	2/5343 (0.0%)
All	All	0.44	1/23760 (0.0%)	0.67	18/32058 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	3
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	59	CYS	CB-SG	5.46	1.91	1.82

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	ARG	NE-CZ-NH1	-21.01	109.80	120.30
1	A	221	ARG	NE-CZ-NH1	-20.91	109.85	120.30
1	C	443	ARG	NE-CZ-NH1	-20.25	110.17	120.30
1	C	46	ARG	NE-CZ-NH2	19.72	130.16	120.30
1	C	443	ARG	NE-CZ-NH2	19.59	130.09	120.30
1	B	367	ARG	NE-CZ-NH1	-19.51	110.55	120.30
1	A	221	ARG	NE-CZ-NH2	18.90	129.75	120.30
1	B	367	ARG	NE-CZ-NH2	17.27	128.93	120.30
1	C	46	ARG	CD-NE-CZ	9.90	137.47	123.60
1	A	221	ARG	CD-NE-CZ	9.66	137.12	123.60
1	C	443	ARG	CD-NE-CZ	9.54	136.95	123.60
1	B	367	ARG	CD-NE-CZ	7.90	134.66	123.60
1	F	443	ARG	NE-CZ-NH1	-7.15	116.73	120.30
1	D	221	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	D	221	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	221	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	E	221	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	F	221	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	433	PRO	Peptide
1	A	91	THR	Mainchain,Peptide
1	B	433	PRO	Peptide
1	C	433	PRO	Peptide
1	D	433	PRO	Peptide
1	E	433	PRO	Peptide
1	F	433	PRO	Peptide
1	F	91	THR	Mainchain,Peptide

## 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	3876	0	3843	65	0
1	B	3876	0	3843	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3876	0	3843	86	0
1	D	3876	0	3843	95	0
1	E	3876	0	3843	91	0
1	F	3876	0	3843	87	0
2	A	5	0	0	2	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	15	0	0	3	0
2	E	15	0	0	1	0
2	F	20	0	0	2	0
3	A	31	0	0	7	0
3	B	51	0	0	14	0
3	C	46	0	0	13	0
3	D	49	0	0	18	0
3	E	47	0	0	14	0
3	F	36	0	0	12	0
All	All	23591	0	23058	485	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 10.

All (485) 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:C:370:MET:SD	3:C:746:HOH:O	2.01	1.18
1:B:227:ILE:O	3:B:702:HOH:O	1.85	0.94
1:E:58:PRO:O	3:E:701:HOH:O	1.85	0.94
1:B:315:GLU:OE2	3:B:701:HOH:O	1.84	0.93
1:F:478:GLY:N	3:F:2101:HOH:O	2.00	0.92
1:D:433:PRO:HA	1:E:420:SER:HB3	1.51	0.92
1:B:88:GLN:OE1	3:B:703:HOH:O	1.88	0.91
1:F:59:CYS:SG	3:F:2130:HOH:O	2.14	0.90
1:B:177:GLU:OE1	3:B:704:HOH:O	1.91	0.89
1:D:88:GLN:OE1	3:D:702:HOH:O	1.92	0.88
1:D:72:ASP:OD2	3:D:701:HOH:O	1.92	0.88
1:B:433:PRO:HA	1:F:420:SER:HB3	1.54	0.88
1:F:59:CYS:SG	3:F:2120:HOH:O	2.28	0.86
1:D:462:GLU:OE2	3:D:703:HOH:O	1.95	0.84
1:D:10:ASP:N	3:D:706:HOH:O	2.12	0.83
1:D:43:GLU:HG2	1:D:44:GLN:HG2	1.60	0.82
1:E:43:GLU:HG2	1:E:44:GLN:HG2	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PHE:HB2	3:B:702:HOH:O	1.81	0.81
1:A:43:GLU:HG2	1:A:44:GLN:HG2	1.62	0.81
1:C:43:GLU:HG2	1:C:44:GLN:HG2	1.62	0.81
1:A:467:GLN:O	3:A:1101:HOH:O	1.99	0.80
1:B:177:GLU:HG2	3:B:727:HOH:O	1.82	0.79
1:D:433:PRO:HA	1:E:420:SER:CB	2.12	0.78
1:F:281:ASP:HB2	1:F:306:LEU:HD11	1.65	0.78
1:B:43:GLU:HG2	1:B:44:GLN:HG2	1.63	0.78
2:F:2003:PO4:O4	3:F:2102:HOH:O	2.01	0.77
1:B:433:PRO:HA	1:F:420:SER:CB	2.14	0.77
1:D:386:TYR:OH	3:D:704:HOH:O	2.03	0.76
1:C:281:ASP:HB2	1:C:306:LEU:HD11	1.68	0.76
1:A:281:ASP:HB2	1:A:306:LEU:HD11	1.67	0.76
1:C:320:GLU:OE1	1:C:342:ARG:NH2	2.18	0.76
1:C:408:ASP:OD2	3:C:702:HOH:O	2.04	0.76
1:F:43:GLU:HG2	1:F:44:GLN:HG2	1.65	0.76
1:E:281:ASP:HB2	1:E:306:LEU:HD11	1.69	0.73
1:D:281:ASP:HB2	1:D:306:LEU:HD11	1.70	0.73
1:C:286:ASN:ND2	3:C:701:HOH:O	2.02	0.72
1:D:80:GLU:OE1	3:D:705:HOH:O	2.06	0.72
1:B:320:GLU:OE1	1:B:342:ARG:NH2	2.23	0.72
1:B:281:ASP:HB2	1:B:306:LEU:HD11	1.71	0.72
1:E:265:ARG:HD3	3:E:706:HOH:O	1.90	0.72
1:A:233:GLU:HG2	1:A:236:TYR:HD2	1.55	0.71
1:B:478:GLY:N	3:B:708:HOH:O	2.23	0.71
1:E:77:GLU:OE1	3:E:703:HOH:O	2.08	0.71
1:C:233:GLU:HG2	1:C:236:TYR:HD2	1.54	0.71
1:E:291:ASP:OD2	3:E:704:HOH:O	2.09	0.71
1:F:229:ASN:O	3:F:2103:HOH:O	2.09	0.71
1:E:71:ARG:NH1	3:E:708:HOH:O	2.23	0.70
1:A:59:CYS:SG	3:A:1126:HOH:O	2.17	0.70
1:C:118:LYS:NZ	1:C:378:ASN:OD1	2.25	0.70
1:E:250:THR:HG22	1:E:273:LYS:HB3	1.72	0.70
1:C:392:ASN:O	3:C:706:HOH:O	2.09	0.70
1:B:150:ARG:NH2	1:B:185:ASP:OD2	2.25	0.70
1:C:269:ARG:O	3:C:705:HOH:O	2.09	0.70
1:E:150:ARG:NH2	1:E:185:ASP:OD2	2.25	0.70
1:F:250:THR:HG22	1:F:273:LYS:HB3	1.73	0.70
1:A:407:ARG:NH1	3:A:1106:HOH:O	2.25	0.69
1:B:243:THR:O	1:B:249:LYS:NZ	2.19	0.69
2:A:1001:PO4:O2	3:A:1102:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:THR:HG22	1:D:273:LYS:HB3	1.75	0.69
1:F:150:ARG:NH2	1:F:185:ASP:OD2	2.25	0.69
1:A:250:THR:HG22	1:A:273:LYS:HB3	1.73	0.69
1:A:320:GLU:OE1	1:A:342:ARG:NH2	2.26	0.68
1:E:233:GLU:HG2	1:E:236:TYR:HD2	1.58	0.68
1:F:233:GLU:HG2	1:F:236:TYR:HD2	1.56	0.68
1:F:320:GLU:OE1	1:F:342:ARG:NH2	2.26	0.68
2:A:1001:PO4:O3	3:A:1103:HOH:O	2.11	0.68
1:D:233:GLU:HG2	1:D:236:TYR:HD2	1.58	0.68
1:D:320:GLU:OE1	1:D:342:ARG:NH2	2.27	0.68
1:F:407:ARG:NH1	3:F:2108:HOH:O	2.26	0.68
1:D:23:ARG:NH2	3:D:709:HOH:O	2.17	0.68
1:F:146:GLU:OE2	1:F:150:ARG:NH1	2.27	0.67
1:E:320:GLU:OE1	1:E:342:ARG:NH2	2.28	0.67
1:C:250:THR:HG22	1:C:273:LYS:HB3	1.77	0.67
1:C:269:ARG:HG2	3:C:705:HOH:O	1.93	0.67
1:E:175:THR:O	3:E:705:HOH:O	2.11	0.67
1:B:233:GLU:HG2	1:B:236:TYR:HD2	1.58	0.67
1:B:146:GLU:OE2	1:B:150:ARG:NH1	2.29	0.66
1:B:55:ILE:O	3:B:705:HOH:O	2.13	0.66
1:B:443:ARG:NH1	3:B:707:HOH:O	2.21	0.65
1:A:150:ARG:NH2	1:A:185:ASP:OD2	2.29	0.65
2:D:603:PO4:O2	3:D:708:HOH:O	2.14	0.64
1:B:68:PRO:HB3	1:D:55:ILE:HG12	1.80	0.64
1:B:250:THR:HG22	1:B:273:LYS:HB3	1.78	0.64
1:C:150:ARG:NH2	1:C:185:ASP:OD2	2.31	0.64
1:E:146:GLU:OE2	1:E:150:ARG:NH1	2.30	0.63
1:B:491:GLU:OE1	3:B:706:HOH:O	2.15	0.63
1:E:221:ARG:NE	3:E:702:HOH:O	2.02	0.63
1:B:431:THR:HG22	1:B:433:PRO:HD3	1.80	0.63
1:D:146:GLU:OE2	1:D:150:ARG:NH1	2.31	0.63
1:A:146:GLU:OE2	1:A:150:ARG:NH1	2.32	0.62
1:F:442:ASP:OD1	3:F:2104:HOH:O	2.16	0.62
1:E:431:THR:HG22	1:E:433:PRO:HD3	1.82	0.61
1:C:416:SER:OG	1:E:436:PRO:HA	2.00	0.61
1:C:146:GLU:OE2	1:C:150:ARG:NH1	2.34	0.61
1:D:150:ARG:NH2	1:D:185:ASP:OD2	2.32	0.61
1:F:480:ASP:HB3	3:F:2101:HOH:O	2.00	0.61
1:C:286:ASN:ND2	1:C:310:LYS:O	2.27	0.61
1:A:277:VAL:HG21	1:A:295:LEU:HD21	1.83	0.60
1:A:502:VAL:HB	1:E:76:TRP:CH2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:SER:HA	1:F:437:THR:HG23	1.84	0.60
1:C:277:VAL:HG21	1:C:295:LEU:HD21	1.83	0.60
1:D:277:VAL:HG21	1:D:295:LEU:HD21	1.82	0.60
1:C:247:GLY:N	3:C:712:HOH:O	2.33	0.60
1:D:431:THR:HG22	1:D:433:PRO:HD3	1.83	0.60
1:E:296:GLU:OE1	3:E:706:HOH:O	2.16	0.60
1:B:277:VAL:HG21	1:B:295:LEU:HD21	1.83	0.59
1:C:190:THR:OG1	1:C:191:ILE:N	2.35	0.59
1:C:323:CYS:O	1:C:345:ALA:HA	2.02	0.59
1:F:277:VAL:HG21	1:F:295:LEU:HD21	1.83	0.59
1:E:277:VAL:HG21	1:E:295:LEU:HD21	1.84	0.59
1:D:190:THR:OG1	1:D:191:ILE:N	2.36	0.59
1:E:266:TYR:OH	2:E:602:PO4:O4	2.15	0.58
1:D:95:GLY:HA3	1:D:129:ALA:O	2.03	0.58
1:E:197:ASN:ND2	3:E:720:HOH:O	2.37	0.57
1:B:414:LEU:HB3	1:B:434:ILE:HA	1.86	0.57
1:E:414:LEU:HB3	1:E:434:ILE:HA	1.85	0.57
1:F:109:LYS:HB3	3:F:2130:HOH:O	2.03	0.57
1:B:434:ILE:HG23	1:B:435:VAL:H	1.69	0.57
1:C:243:THR:O	1:C:249:LYS:NZ	2.23	0.57
1:A:431:THR:HG22	1:A:433:PRO:HD3	1.86	0.57
1:C:414:LEU:HB3	1:C:434:ILE:HA	1.87	0.57
1:D:243:THR:O	1:D:249:LYS:NZ	2.27	0.57
1:F:190:THR:OG1	1:F:191:ILE:N	2.38	0.57
1:A:286:ASN:ND2	1:A:310:LYS:O	2.28	0.57
1:A:135:ILE:HG13	1:A:140:TYR:CE1	2.40	0.57
1:E:135:ILE:HG13	1:E:140:TYR:CE1	2.40	0.56
1:D:54:ARG:NH2	3:D:707:HOH:O	2.14	0.56
1:D:414:LEU:HB3	1:D:434:ILE:HA	1.87	0.56
1:E:434:ILE:HG23	1:E:435:VAL:H	1.69	0.56
1:A:414:LEU:HB3	1:A:434:ILE:HA	1.88	0.56
1:C:135:ILE:HG13	1:C:140:TYR:CE1	2.40	0.56
1:D:118:LYS:NZ	1:D:378:ASN:OD1	2.39	0.56
1:F:12:ASN:O	1:F:14:PHE:N	2.39	0.56
1:F:434:ILE:HG23	1:F:435:VAL:H	1.71	0.56
1:B:95:GLY:HA3	1:B:129:ALA:O	2.05	0.56
1:C:151:ARG:NH1	1:F:503:THR:HG23	2.21	0.56
1:E:34:GLU:HA	1:E:37:ARG:O	2.06	0.55
1:F:135:ILE:HG13	1:F:140:TYR:CE1	2.41	0.55
1:E:470:ARG:HA	1:E:473:MET:HE2	1.88	0.55
1:F:118:LYS:NZ	1:F:378:ASN:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:THR:HG23	1:F:151:ARG:HH11	1.72	0.55
1:C:34:GLU:HA	1:C:37:ARG:O	2.07	0.55
1:A:470:ARG:HA	1:A:473:MET:HE2	1.89	0.55
1:E:190:THR:OG1	1:E:191:ILE:N	2.40	0.55
1:D:12:ASN:C	1:D:14:PHE:H	2.11	0.54
1:E:62:VAL:HG21	1:E:109:LYS:HD3	1.89	0.54
1:F:431:THR:HG22	1:F:433:PRO:HD3	1.88	0.54
1:A:95:GLY:HA3	1:A:129:ALA:O	2.07	0.54
1:C:416:SER:HA	1:E:437:THR:HG23	1.89	0.54
1:D:63:LEU:HD21	1:D:65:LEU:HD21	1.90	0.54
1:D:470:ARG:HA	1:D:473:MET:HE2	1.88	0.54
1:F:146:GLU:O	1:F:150:ARG:HG3	2.07	0.54
1:B:34:GLU:HA	1:B:37:ARG:O	2.07	0.54
1:A:243:THR:O	1:A:249:LYS:NZ	2.28	0.54
1:B:339:ASN:OD1	1:B:339:ASN:N	2.35	0.54
1:D:179:GLU:OE1	3:D:710:HOH:O	2.18	0.54
1:B:319:LEU:HD12	1:B:319:LEU:H	1.73	0.54
1:F:12:ASN:C	1:F:14:PHE:H	2.11	0.54
1:B:59:CYS:SG	3:B:744:HOH:O	2.15	0.54
1:B:76:TRP:O	3:D:707:HOH:O	2.19	0.54
1:D:323:CYS:O	1:D:345:ALA:HA	2.08	0.54
1:B:12:ASN:C	1:B:14:PHE:H	2.11	0.54
1:B:12:ASN:O	1:B:14:PHE:N	2.41	0.54
1:D:51:GLY:HA2	3:D:707:HOH:O	2.07	0.54
1:F:323:CYS:O	1:F:345:ALA:HA	2.08	0.54
1:E:323:CYS:O	1:E:345:ALA:HA	2.08	0.54
1:B:76:TRP:CH2	1:D:502:VAL:HB	2.44	0.53
1:C:95:GLY:HA3	1:C:129:ALA:O	2.08	0.53
1:D:146:GLU:O	1:D:150:ARG:HG3	2.08	0.53
1:A:152:PHE:CE2	1:A:156:LEU:HD11	2.43	0.53
1:C:71:ARG:HD2	1:C:77:GLU:OE2	2.09	0.53
1:D:135:ILE:HG13	1:D:140:TYR:CE1	2.44	0.53
1:A:118:LYS:NZ	1:A:378:ASN:OD1	2.41	0.53
1:C:233:GLU:HG2	1:C:236:TYR:CD2	2.41	0.53
1:A:12:ASN:C	1:A:14:PHE:H	2.12	0.53
1:C:420:SER:HB3	1:E:433:PRO:HA	1.91	0.53
1:C:478:GLY:N	3:C:703:HOH:O	2.07	0.53
1:D:116:THR:O	3:D:711:HOH:O	2.19	0.53
1:E:12:ASN:C	1:E:14:PHE:H	2.11	0.53
1:F:34:GLU:HA	1:F:37:ARG:O	2.08	0.53
1:E:95:GLY:HA3	1:E:129:ALA:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:LYS:NZ	1:E:378:ASN:OD1	2.41	0.53
1:D:501:GLY:O	1:D:502:VAL:HG23	2.09	0.53
1:B:323:CYS:O	1:B:345:ALA:HA	2.09	0.52
1:D:407:ARG:NH1	3:D:718:HOH:O	2.41	0.52
1:F:414:LEU:HB3	1:F:434:ILE:HA	1.91	0.52
1:D:213:HIS:HD1	2:D:601:PO4:P	2.31	0.52
1:E:63:LEU:HD21	1:E:65:LEU:HD21	1.91	0.52
1:E:70:ARG:HD3	1:E:76:TRP:CZ2	2.45	0.52
1:E:173:MET:N	3:E:705:HOH:O	2.28	0.52
1:F:95:GLY:HA3	1:F:129:ALA:O	2.09	0.52
1:F:70:ARG:HD3	1:F:76:TRP:CZ2	2.44	0.52
1:F:470:ARG:HA	1:F:473:MET:HE2	1.91	0.52
1:B:39:ARG:HG3	1:B:40:GLU:HB3	1.90	0.52
1:A:190:THR:OG1	1:A:191:ILE:N	2.39	0.52
1:A:323:CYS:O	1:A:345:ALA:HA	2.10	0.52
1:C:62:VAL:HG21	1:C:109:LYS:HD3	1.91	0.52
1:C:12:ASN:C	1:C:14:PHE:H	2.12	0.52
1:D:434:ILE:HG23	1:D:435:VAL:H	1.74	0.52
1:A:34:GLU:HA	1:A:37:ARG:O	2.09	0.52
1:C:431:THR:HG22	1:C:433:PRO:HD3	1.92	0.52
1:D:286:ASN:ND2	1:D:310:LYS:O	2.31	0.52
1:E:501:GLY:O	1:E:502:VAL:HG23	2.10	0.52
1:B:63:LEU:HD21	1:B:65:LEU:HD21	1.92	0.52
1:C:470:ARG:HA	1:C:473:MET:HE2	1.91	0.52
1:D:39:ARG:HG3	1:D:40:GLU:HB3	1.92	0.52
1:B:70:ARG:HD3	1:B:76:TRP:CZ2	2.45	0.52
1:B:135:ILE:HG13	1:B:140:TYR:CE1	2.45	0.52
1:B:501:GLY:O	1:B:502:VAL:HG23	2.10	0.52
1:E:39:ARG:HG3	1:E:40:GLU:HB3	1.92	0.52
1:C:135:ILE:HD12	1:C:148:ILE:HD13	1.92	0.51
1:C:437:THR:HG23	1:D:416:SER:HA	1.92	0.51
1:D:12:ASN:O	1:D:14:PHE:N	2.42	0.51
1:D:34:GLU:HA	1:D:37:ARG:O	2.09	0.51
1:D:152:PHE:CE2	1:D:156:LEU:HD11	2.45	0.51
1:E:152:PHE:CE2	1:E:156:LEU:HD11	2.45	0.51
1:E:12:ASN:O	1:E:14:PHE:N	2.43	0.51
1:C:279:GLU:OE2	1:C:299:LYS:NZ	2.43	0.51
1:D:71:ARG:HD2	1:D:77:GLU:OE2	2.10	0.51
1:B:436:PRO:HA	1:F:416:SER:OG	2.09	0.51
1:B:64:SER:HB2	1:D:62:VAL:HB	1.93	0.51
1:B:76:TRP:HB2	1:D:51:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HD13	1:B:348:ILE:HD13	1.91	0.51
1:F:233:GLU:HG2	1:F:236:TYR:CD2	2.43	0.51
1:A:12:ASN:O	1:A:14:PHE:N	2.44	0.51
1:A:151:ARG:NH1	1:E:503:THR:HG23	2.26	0.51
1:D:339:ASN:OD1	1:D:339:ASN:N	2.38	0.51
1:F:71:ARG:HD2	1:F:77:GLU:OE2	2.11	0.51
1:F:152:PHE:CE2	1:F:156:LEU:HD11	2.46	0.51
1:B:118:LYS:NZ	1:B:378:ASN:OD1	2.42	0.51
1:B:190:THR:OG1	1:B:191:ILE:N	2.44	0.51
1:C:12:ASN:O	1:C:14:PHE:N	2.44	0.51
1:C:434:ILE:HG23	1:C:435:VAL:H	1.76	0.50
1:E:146:GLU:O	1:E:150:ARG:HG3	2.12	0.50
1:F:62:VAL:HG21	1:F:109:LYS:HD3	1.94	0.50
1:B:470:ARG:HA	1:B:473:MET:HE2	1.94	0.50
1:F:501:GLY:O	1:F:502:VAL:HG23	2.12	0.50
1:A:39:ARG:HG3	1:A:40:GLU:HB3	1.93	0.50
1:C:39:ARG:HG3	1:C:40:GLU:HB3	1.93	0.50
1:A:279:GLU:OE2	1:A:299:LYS:NZ	2.44	0.50
1:F:286:ASN:ND2	1:F:310:LYS:O	2.30	0.50
1:C:480:ASP:HB3	3:C:703:HOH:O	2.12	0.50
1:D:335:LEU:HD13	1:D:348:ILE:HD13	1.94	0.50
1:C:503:THR:HG23	1:F:151:ARG:NH1	2.25	0.50
1:D:59:CYS:HA	1:D:86:HIS:HA	1.94	0.50
1:A:70:ARG:CZ	1:E:505:THR:HB	2.41	0.50
1:C:146:GLU:O	1:C:150:ARG:HG3	2.12	0.49
1:E:319:LEU:HD12	1:E:319:LEU:H	1.77	0.49
1:B:146:GLU:O	1:B:150:ARG:HG3	2.12	0.49
1:A:501:GLY:O	1:A:502:VAL:HG23	2.12	0.49
1:C:152:PHE:CE2	1:C:156:LEU:HD11	2.47	0.49
1:F:239:ILE:HG21	1:F:479:LEU:HD21	1.94	0.49
1:A:63:LEU:HD21	1:A:65:LEU:HD21	1.93	0.49
1:B:285:TRP:HE1	1:B:287:PRO:HG3	1.77	0.49
1:B:480:ASP:N	3:B:708:HOH:O	2.45	0.49
1:A:335:LEU:HD13	1:A:348:ILE:HD13	1.95	0.49
1:C:151:ARG:HH11	1:F:503:THR:HG23	1.77	0.49
1:F:238:SER:O	1:F:241:GLY:N	2.40	0.49
1:A:285:TRP:HE1	1:A:287:PRO:HG3	1.77	0.49
1:E:335:LEU:HD13	1:E:348:ILE:HD13	1.94	0.49
1:A:233:GLU:HG2	1:A:236:TYR:CD2	2.41	0.49
1:F:339:ASN:OD1	1:F:339:ASN:N	2.41	0.49
1:C:70:ARG:HD3	1:C:76:TRP:CZ2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG21	1:A:109:LYS:HD3	1.94	0.48
1:D:70:ARG:HD3	1:D:76:TRP:CZ2	2.48	0.48
1:B:62:VAL:HG21	1:B:109:LYS:HD3	1.96	0.48
1:F:486:TYR:OH	3:F:2105:HOH:O	2.18	0.48
1:C:249:LYS:HD3	1:C:249:LYS:N	2.28	0.48
1:A:434:ILE:HG23	1:A:435:VAL:H	1.78	0.48
1:B:265:ARG:NH2	2:B:602:PO4:O2	2.45	0.48
1:B:279:GLU:OE2	1:B:299:LYS:NZ	2.45	0.48
1:E:286:ASN:ND2	1:E:310:LYS:O	2.32	0.48
1:F:285:TRP:HE1	1:F:287:PRO:HG3	1.79	0.48
1:B:336:THR:HG23	1:B:338:SER:H	1.78	0.48
1:B:59:CYS:HA	1:B:86:HIS:HA	1.95	0.48
1:B:70:ARG:NH2	1:E:143:ASN:OD1	2.48	0.47
1:B:400:ARG:O	1:B:400:ARG:HG3	2.14	0.47
1:E:78:VAL:HG23	3:E:721:HOH:O	2.12	0.47
1:F:266:TYR:OH	2:F:2002:PO4:O4	2.31	0.47
1:A:400:ARG:O	1:A:400:ARG:HG3	2.13	0.47
1:C:501:GLY:O	1:C:502:VAL:HG23	2.14	0.47
1:D:62:VAL:HG21	1:D:109:LYS:HD3	1.96	0.47
1:F:39:ARG:HG3	1:F:40:GLU:HB3	1.96	0.47
1:A:71:ARG:HD2	1:A:77:GLU:OE2	2.15	0.47
1:D:378:ASN:HA	3:D:724:HOH:O	2.14	0.47
1:C:456:GLY:HA3	1:D:401:LEU:HD23	1.95	0.47
1:F:32:LEU:O	1:F:37:ARG:HB3	2.15	0.47
1:F:335:LEU:HD13	1:F:348:ILE:HD13	1.96	0.47
1:B:71:ARG:HD2	1:B:77:GLU:OE2	2.15	0.47
1:C:45:LYS:HD2	1:C:45:LYS:HA	1.68	0.47
1:D:95:GLY:O	1:D:169:PRO:HA	2.15	0.47
1:E:339:ASN:OD1	1:E:339:ASN:N	2.39	0.47
1:B:326:LEU:O	1:B:328:PRO:HD3	2.15	0.47
1:E:95:GLY:O	1:E:169:PRO:HA	2.15	0.47
1:B:95:GLY:O	1:B:169:PRO:HA	2.14	0.47
1:C:420:SER:CB	1:E:433:PRO:HA	2.44	0.47
1:C:463:ARG:NH2	2:D:603:PO4:O4	2.47	0.46
1:B:233:GLU:HG2	1:B:236:TYR:CD2	2.45	0.46
1:D:462:GLU:CD	3:D:703:HOH:O	2.49	0.46
1:A:95:GLY:O	1:A:169:PRO:HA	2.15	0.46
1:B:340:ALA:HB3	1:B:341:PRO:HD3	1.97	0.46
1:C:60:ASN:OD1	3:C:707:HOH:O	2.20	0.46
1:C:111:LEU:HD13	1:C:130:LYS:HE3	1.98	0.46
1:B:286:ASN:ND2	1:B:310:LYS:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:GLU:OE2	1:B:482:ARG:NH2	2.49	0.46
1:D:233:GLU:HG2	1:D:236:TYR:CD2	2.45	0.46
1:D:413:LEU:HD13	1:E:413:LEU:HD13	1.97	0.46
1:C:285:TRP:HE1	1:C:287:PRO:HG3	1.80	0.46
1:D:434:ILE:O	1:E:420:SER:OG	2.33	0.46
1:E:41:SER:HB2	1:E:45:LYS:NZ	2.31	0.46
1:A:436:PRO:HB3	1:A:440:PHE:CD2	2.51	0.46
1:C:400:ARG:O	1:C:400:ARG:HG3	2.16	0.46
1:C:95:GLY:O	1:C:169:PRO:HA	2.16	0.45
1:D:32:LEU:O	1:D:37:ARG:HB3	2.15	0.45
1:A:70:ARG:HD3	1:A:76:TRP:CZ2	2.51	0.45
1:E:71:ARG:HD2	1:E:77:GLU:OE2	2.17	0.45
1:D:45:LYS:HD2	1:D:45:LYS:HA	1.67	0.45
1:D:340:ALA:HB3	1:D:341:PRO:HD3	1.99	0.45
1:B:460:THR:HA	3:B:730:HOH:O	2.16	0.45
1:C:252:VAL:HG13	1:C:276:ALA:HB3	1.99	0.45
1:C:336:THR:HG23	1:C:338:SER:H	1.81	0.45
1:D:285:TRP:HE1	1:D:287:PRO:HG3	1.80	0.45
1:E:279:GLU:OE2	1:E:299:LYS:NZ	2.46	0.45
1:B:319:LEU:HD12	1:B:319:LEU:N	2.32	0.45
1:E:59:CYS:HA	1:E:86:HIS:HA	1.98	0.45
1:F:428:HIS:HD2	3:F:2112:HOH:O	1.99	0.45
1:C:21:PHE:CE2	1:C:57:LYS:HB2	2.52	0.45
1:E:277:VAL:HG23	1:E:305:ILE:HD12	1.97	0.45
1:C:443:ARG:NH2	1:D:409:SER:OG	2.50	0.45
1:D:281:ASP:HB2	1:D:282:GLY:H	1.61	0.45
1:C:273:LYS:HD2	3:C:722:HOH:O	2.17	0.45
1:A:336:THR:HG23	1:A:338:SER:H	1.81	0.44
1:D:239:ILE:HG21	1:D:479:LEU:HD21	1.98	0.44
1:F:95:GLY:O	1:F:169:PRO:HA	2.16	0.44
1:B:505:THR:HB	1:D:70:ARG:NH2	2.32	0.44
1:C:32:LEU:O	1:C:37:ARG:HB3	2.17	0.44
1:E:326:LEU:O	1:E:328:PRO:HD3	2.18	0.44
1:A:433:PRO:HA	1:B:420:SER:HB3	2.00	0.44
1:E:265:ARG:CD	3:E:706:HOH:O	2.58	0.44
1:F:21:PHE:CE2	1:F:57:LYS:HB2	2.53	0.44
1:A:32:LEU:O	1:A:37:ARG:HB3	2.17	0.44
1:B:45:LYS:HD2	1:B:45:LYS:HA	1.68	0.44
1:C:319:LEU:HD12	1:C:319:LEU:H	1.83	0.44
1:B:187:TYR:CE2	1:B:192:GLY:HA3	2.53	0.44
1:D:242:MET:HE2	1:D:249:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:LEU:HB3	3:B:708:HOH:O	2.17	0.44
1:F:63:LEU:HD21	1:F:65:LEU:HD21	2.00	0.44
1:E:265:ARG:HG2	3:E:716:HOH:O	2.18	0.43
1:D:504:PHE:CZ	1:E:186:THR:HG23	2.53	0.43
1:E:340:ALA:HB3	1:E:341:PRO:HD3	1.98	0.43
1:F:71:ARG:HE	1:F:71:ARG:HB3	1.68	0.43
1:A:249:LYS:HD3	1:A:249:LYS:N	2.32	0.43
1:B:434:ILE:O	1:F:420:SER:OG	2.30	0.43
1:D:429:GLY:HA3	3:D:719:HOH:O	2.17	0.43
1:A:60:ASN:OD1	3:A:1104:HOH:O	2.21	0.43
1:B:375:LEU:HD12	1:B:375:LEU:HA	1.84	0.43
1:F:314:TYR:CE2	1:F:318:ILE:HA	2.53	0.43
1:B:143:ASN:OD1	1:E:70:ARG:NH2	2.52	0.43
1:D:350:GLU:OE1	1:D:482:ARG:NH2	2.50	0.43
1:E:32:LEU:O	1:E:37:ARG:HB3	2.19	0.43
1:F:261:LEU:HD11	3:F:2111:HOH:O	2.17	0.43
1:F:281:ASP:HB2	1:F:282:GLY:H	1.58	0.43
1:B:152:PHE:CE2	1:B:156:LEU:HD11	2.54	0.43
1:C:63:LEU:HD21	1:C:65:LEU:HD21	1.99	0.43
1:C:310:LYS:HG2	3:C:701:HOH:O	2.19	0.43
1:D:111:LEU:HD13	1:D:130:LYS:HE3	2.01	0.43
1:D:187:TYR:CE2	1:D:192:GLY:HA3	2.53	0.43
1:F:277:VAL:HG23	1:F:305:ILE:HD12	2.01	0.43
1:A:146:GLU:O	1:A:150:ARG:HG3	2.18	0.43
1:A:314:TYR:CE2	1:A:318:ILE:HA	2.54	0.43
1:D:436:PRO:HA	1:E:416:SER:OG	2.19	0.43
1:F:164:PRO:HG2	1:F:195:ASP:OD2	2.19	0.43
1:A:416:SER:OG	1:F:436:PRO:HA	2.18	0.43
1:B:41:SER:HB2	1:B:45:LYS:NZ	2.34	0.43
1:C:314:TYR:CE2	1:C:318:ILE:HA	2.53	0.43
1:C:474:LYS:NZ	1:C:491:GLU:OE2	2.52	0.43
1:D:279:GLU:OE2	1:D:299:LYS:NZ	2.48	0.43
1:F:253:VAL:O	1:F:277:VAL:HA	2.19	0.43
1:B:32:LEU:O	1:B:37:ARG:HB3	2.19	0.43
1:C:159:LYS:HE3	1:F:61:HIS:CD2	2.54	0.43
1:C:335:LEU:HD13	1:C:348:ILE:HD13	2.00	0.43
1:E:427:LYS:NZ	3:E:712:HOH:O	2.29	0.43
1:B:304:SER:OG	1:B:305:ILE:N	2.52	0.42
1:B:413:LEU:HD13	1:F:413:LEU:HD13	2.01	0.42
1:E:285:TRP:HE1	1:E:287:PRO:HG3	1.84	0.42
1:E:319:LEU:HD12	1:E:319:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:ARG:HE	1:C:470:ARG:HB2	1.70	0.42
1:F:336:THR:HG23	1:F:338:SER:H	1.85	0.42
1:A:187:TYR:CE2	1:A:192:GLY:HA3	2.54	0.42
1:E:111:LEU:HD13	1:E:130:LYS:HE3	2.00	0.42
1:F:436:PRO:HB3	1:F:440:PHE:CD2	2.55	0.42
1:A:59:CYS:HA	1:A:86:HIS:HA	2.00	0.42
1:A:277:VAL:HG23	1:A:305:ILE:HD12	2.01	0.42
1:B:21:PHE:CE2	1:B:57:LYS:HB2	2.54	0.42
1:B:94:LYS:HD2	1:B:168:VAL:HB	2.01	0.42
1:B:470:ARG:HE	1:B:470:ARG:HB2	1.69	0.42
1:C:412:HIS:HB3	1:E:440:PHE:CG	2.54	0.42
1:D:171:PRO:HG3	1:D:180:MET:HG3	2.02	0.42
1:E:21:PHE:CE2	1:E:57:LYS:HB2	2.55	0.42
1:F:279:GLU:OE2	1:F:299:LYS:NZ	2.49	0.42
1:D:249:LYS:N	1:D:249:LYS:HD3	2.34	0.42
1:F:41:SER:HB2	1:F:45:LYS:NZ	2.35	0.42
1:F:133:VAL:O	1:F:135:ILE:HG22	2.20	0.42
1:A:304:SER:OG	1:A:305:ILE:N	2.53	0.42
1:D:326:LEU:O	1:D:328:PRO:HD3	2.20	0.42
1:B:135:ILE:HD12	1:B:148:ILE:HD13	2.00	0.42
1:B:253:VAL:O	1:B:277:VAL:HA	2.20	0.42
1:C:43:GLU:N	1:C:43:GLU:OE1	2.53	0.42
1:C:350:GLU:OE1	1:C:482:ARG:NH2	2.52	0.42
1:F:135:ILE:HD12	1:F:148:ILE:HD13	2.01	0.42
1:A:70:ARG:NH2	1:E:505:THR:HB	2.35	0.42
1:F:111:LEU:HD13	1:F:130:LYS:HE3	2.02	0.42
1:F:249:LYS:HD3	1:F:249:LYS:N	2.35	0.42
1:A:43:GLU:OE1	1:A:43:GLU:N	2.53	0.41
1:E:336:THR:HG23	1:E:338:SER:H	1.83	0.41
1:F:69:ILE:HG12	1:F:79:ILE:HD11	2.02	0.41
1:A:253:VAL:O	1:A:277:VAL:HA	2.20	0.41
1:B:93:CYS:HB3	1:B:129:ALA:HB2	2.02	0.41
1:C:239:ILE:HG21	1:C:479:LEU:HD21	2.02	0.41
1:D:427:LYS:HB2	1:D:428:HIS:H	1.72	0.41
1:E:77:GLU:OE1	1:E:140:TYR:OH	2.30	0.41
1:E:94:LYS:HD2	1:E:168:VAL:HB	2.02	0.41
1:E:503:THR:HB	1:E:504:PHE:H	1.66	0.41
1:D:93:CYS:HB3	1:D:129:ALA:HB2	2.03	0.41
1:B:427:LYS:HB2	1:B:428:HIS:H	1.65	0.41
1:C:412:HIS:HB3	1:E:440:PHE:CD1	2.56	0.41
1:F:243:THR:O	1:F:249:LYS:NZ	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:PRO:HB3	1:D:440:PHE:CD2	2.55	0.41
1:E:314:TYR:CE2	1:E:318:ILE:HA	2.55	0.41
1:A:252:VAL:HG13	1:A:276:ALA:HB3	2.03	0.41
1:A:340:ALA:HB3	1:A:341:PRO:HD3	2.03	0.41
1:B:277:VAL:HG23	1:B:305:ILE:HD12	2.03	0.41
1:D:238:SER:O	1:D:241:GLY:N	2.41	0.41
1:D:304:SER:OG	1:D:305:ILE:N	2.53	0.41
1:D:336:THR:HG23	1:D:338:SER:H	1.85	0.41
1:D:375:LEU:HD22	1:D:486:TYR:CE1	2.55	0.41
1:E:474:LYS:NZ	1:E:491:GLU:OE2	2.54	0.41
1:F:94:LYS:HD3	1:F:126:PHE:CE2	2.55	0.41
1:F:356:THR:HG23	1:F:360:ALA:HB3	2.02	0.41
1:F:474:LYS:NZ	1:F:491:GLU:OE2	2.53	0.41
1:A:21:PHE:CE2	1:A:57:LYS:HB2	2.55	0.41
1:C:69:ILE:HG12	1:C:79:ILE:HD11	2.02	0.41
1:E:281:ASP:HB2	1:E:282:GLY:H	1.58	0.41
1:B:111:LEU:HD13	1:B:130:LYS:HE3	2.03	0.41
1:B:314:TYR:CE2	1:B:318:ILE:HA	2.56	0.41
1:B:503:THR:HB	1:B:504:PHE:H	1.68	0.41
1:D:249:LYS:HG3	1:D:324:ASP:CB	2.51	0.41
1:D:359:GLU:HG3	3:D:706:HOH:O	2.20	0.41
1:E:32:LEU:HD12	1:E:32:LEU:HA	1.82	0.41
1:E:135:ILE:HD12	1:E:148:ILE:HD13	2.02	0.41
1:F:94:LYS:HD2	1:F:168:VAL:HB	2.03	0.41
1:F:249:LYS:HG3	1:F:324:ASP:CB	2.51	0.41
1:A:71:ARG:HE	1:A:71:ARG:HB3	1.68	0.41
1:C:94:LYS:HD2	1:C:168:VAL:HB	2.03	0.41
1:D:314:TYR:CE2	1:D:318:ILE:HA	2.56	0.41
1:D:470:ARG:HE	1:D:470:ARG:HB2	1.68	0.41
1:F:275:ILE:HD11	1:F:323:CYS:HB3	2.03	0.41
1:B:71:ARG:HE	1:B:71:ARG:HB3	1.65	0.40
1:C:249:LYS:HG3	1:C:324:ASP:CB	2.51	0.40
1:D:71:ARG:HE	1:D:71:ARG:HB3	1.66	0.40
1:D:375:LEU:HD12	1:D:375:LEU:HA	1.86	0.40
1:E:251:PHE:CZ	1:E:274:CYS:HB2	2.56	0.40
1:B:283:SER:OG	1:B:314:TYR:HB3	2.21	0.40
1:B:474:LYS:NZ	1:B:491:GLU:OE2	2.54	0.40
1:D:37:ARG:NH1	1:D:39:ARG:HB2	2.36	0.40
1:E:71:ARG:HE	1:E:71:ARG:HB3	1.63	0.40
1:F:283:SER:OG	1:F:314:TYR:HB3	2.22	0.40
1:A:111:LEU:HD13	1:A:130:LYS:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1103:HOH:O	1:B:397:SER:OG	2.22	0.40
1:B:310:LYS:HE3	1:B:310:LYS:HB2	1.91	0.40
1:B:319:LEU:H	1:B:319:LEU:CD1	2.33	0.40
1:C:187:TYR:CE2	1:C:192:GLY:HA3	2.57	0.40
1:D:41:SER:HB2	1:D:45:LYS:NZ	2.35	0.40
1:E:45:LYS:HA	1:E:45:LYS:HD2	1.66	0.40
1:A:41:SER:HB2	1:A:45:LYS:NZ	2.36	0.40
1:C:238:SER:O	1:C:241:GLY:N	2.40	0.40
1:C:277:VAL:HG23	1:C:305:ILE:HD12	2.02	0.40
1:D:319:LEU:H	1:D:319:LEU:HD12	1.86	0.40
1:F:427:LYS:HB2	1:F:428:HIS:H	1.66	0.40
1:A:239:ILE:HG21	1:A:479:LEU:HD21	2.02	0.40
1:C:253:VAL:O	1:C:277:VAL:HA	2.22	0.40
1:C:346:LYS:CE	3:C:708:HOH:O	2.69	0.40
1:E:252:VAL:HG13	1:E:276:ALA:HB3	2.03	0.40
1:E:373:PRO:HG3	1:E:482:ARG:HA	2.04	0.40
1:F:400:ARG:O	1:F:400:ARG:HG3	2.21	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	494/496 (100%)	452 (92%)	34 (7%)	8 (2%)	9	24
1	B	494/496 (100%)	453 (92%)	33 (7%)	8 (2%)	9	24
1	C	494/496 (100%)	448 (91%)	36 (7%)	10 (2%)	7	19
1	D	494/496 (100%)	452 (92%)	34 (7%)	8 (2%)	9	24
1	E	494/496 (100%)	455 (92%)	30 (6%)	9 (2%)	8	21
1	F	494/496 (100%)	448 (91%)	37 (8%)	9 (2%)	8	21
All	All	2964/2976 (100%)	2708 (91%)	204 (7%)	52 (2%)	8	21

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	40	GLU
1	A	434	ILE
1	B	35	ASP
1	B	40	GLU
1	B	434	ILE
1	C	35	ASP
1	C	40	GLU
1	C	434	ILE
1	D	35	ASP
1	D	40	GLU
1	D	434	ILE
1	E	35	ASP
1	E	40	GLU
1	E	434	ILE
1	F	35	ASP
1	F	40	GLU
1	F	434	ILE
1	A	13	PHE
1	A	426	GLY
1	A	502	VAL
1	B	13	PHE
1	B	426	GLY
1	B	502	VAL
1	C	13	PHE
1	C	426	GLY
1	C	502	VAL
1	D	13	PHE
1	D	426	GLY
1	D	502	VAL
1	E	13	PHE
1	E	426	GLY
1	E	502	VAL
1	F	13	PHE
1	F	92	PRO
1	F	426	GLY
1	F	502	VAL
1	A	331	SER
1	B	331	SER
1	C	331	SER
1	C	435	VAL
1	D	331	SER

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Mol	Chain	Res	Type
1	E	331	SER
1	F	331	SER
1	F	435	VAL
1	A	435	VAL
1	B	435	VAL
1	D	435	VAL
1	E	172	ASP
1	E	435	VAL
1	C	244	PRO
1	C	239	ILE

### 5.3.2 Protein sidechains [i](#)

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	413/413 (100%)	392 (95%)	21 (5%)	24	50
1	B	413/413 (100%)	391 (95%)	22 (5%)	22	48
1	C	413/413 (100%)	390 (94%)	23 (6%)	21	45
1	D	413/413 (100%)	392 (95%)	21 (5%)	24	50
1	E	413/413 (100%)	393 (95%)	20 (5%)	25	53
1	F	413/413 (100%)	392 (95%)	21 (5%)	24	50
All	All	2478/2478 (100%)	2350 (95%)	128 (5%)	23	49

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	35	ASP
1	A	40	GLU
1	A	45	LYS
1	A	135	ILE
1	A	235	SER
1	A	249	LYS
1	A	267	LEU

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Mol	Chain	Res	Type
1	A	281	ASP
1	A	300	LEU
1	A	306	LEU
1	A	318	ILE
1	A	339	ASN
1	A	342	ARG
1	A	409	SER
1	A	415	MET
1	A	432	ILE
1	A	435	VAL
1	A	455	SER
1	A	470	ARG
1	A	503	THR
1	B	32	LEU
1	B	35	ASP
1	B	40	GLU
1	B	45	LYS
1	B	135	ILE
1	B	235	SER
1	B	249	LYS
1	B	267	LEU
1	B	281	ASP
1	B	300	LEU
1	B	306	LEU
1	B	318	ILE
1	B	339	ASN
1	B	342	ARG
1	B	409	SER
1	B	415	MET
1	B	432	ILE
1	B	435	VAL
1	B	455	SER
1	B	470	ARG
1	B	503	THR
1	B	505	THR
1	C	32	LEU
1	C	35	ASP
1	C	40	GLU
1	C	45	LYS
1	C	46	ARG
1	C	135	ILE
1	C	235	SER

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Mol	Chain	Res	Type
1	C	249	LYS
1	C	267	LEU
1	C	281	ASP
1	C	300	LEU
1	C	306	LEU
1	C	318	ILE
1	C	339	ASN
1	C	342	ARG
1	C	409	SER
1	C	415	MET
1	C	432	ILE
1	C	435	VAL
1	C	443	ARG
1	C	455	SER
1	C	470	ARG
1	C	503	THR
1	D	32	LEU
1	D	35	ASP
1	D	40	GLU
1	D	45	LYS
1	D	135	ILE
1	D	235	SER
1	D	249	LYS
1	D	267	LEU
1	D	281	ASP
1	D	300	LEU
1	D	306	LEU
1	D	318	ILE
1	D	339	ASN
1	D	342	ARG
1	D	409	SER
1	D	415	MET
1	D	432	ILE
1	D	435	VAL
1	D	455	SER
1	D	470	ARG
1	D	503	THR
1	E	32	LEU
1	E	35	ASP
1	E	40	GLU
1	E	45	LYS
1	E	135	ILE

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Mol	Chain	Res	Type
1	E	235	SER
1	E	249	LYS
1	E	267	LEU
1	E	281	ASP
1	E	300	LEU
1	E	306	LEU
1	E	318	ILE
1	E	339	ASN
1	E	342	ARG
1	E	409	SER
1	E	415	MET
1	E	432	ILE
1	E	435	VAL
1	E	455	SER
1	E	503	THR
1	F	32	LEU
1	F	35	ASP
1	F	40	GLU
1	F	45	LYS
1	F	135	ILE
1	F	235	SER
1	F	249	LYS
1	F	267	LEU
1	F	281	ASP
1	F	300	LEU
1	F	306	LEU
1	F	318	ILE
1	F	339	ASN
1	F	342	ARG
1	F	400	ARG
1	F	409	SER
1	F	415	MET
1	F	432	ILE
1	F	435	VAL
1	F	455	SER
1	F	503	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

15 ligands are 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	$\# Z  > 2$
2	PO4	D	601	-	4,4,4	0.89	0	6,6,6	0.33	0
2	PO4	A	1001	-	4,4,4	0.86	0	6,6,6	0.64	0
2	PO4	E	601	-	4,4,4	0.92	0	6,6,6	0.39	0
2	PO4	F	2004	-	4,4,4	0.89	0	6,6,6	0.88	0
2	PO4	F	2003	-	4,4,4	0.85	0	6,6,6	0.45	0
2	PO4	E	602	-	4,4,4	0.96	0	6,6,6	0.44	0
2	PO4	D	603	-	4,4,4	1.04	0	6,6,6	0.76	0
2	PO4	C	602	-	4,4,4	0.94	0	6,6,6	1.33	1 (16%)
2	PO4	E	603	-	4,4,4	0.80	0	6,6,6	0.51	0
2	PO4	C	601	-	4,4,4	0.68	0	6,6,6	0.74	0
2	PO4	F	2001	-	4,4,4	0.74	0	6,6,6	0.61	0
2	PO4	D	602	-	4,4,4	0.74	0	6,6,6	0.52	0
2	PO4	F	2002	-	4,4,4	0.89	0	6,6,6	0.50	0
2	PO4	B	601	-	4,4,4	0.72	0	6,6,6	0.73	0
2	PO4	B	602	-	4,4,4	0.76	0	6,6,6	0.55	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	PO4	O2-P-O1	-2.35	102.63	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	PO4	1	0
2	A	1001	PO4	2	0
2	F	2003	PO4	1	0
2	E	602	PO4	1	0
2	D	603	PO4	2	0
2	F	2002	PO4	1	0
2	B	602	PO4	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	496/496 (100%)	0.53	64 (12%) <b>3</b> <b>2</b>	30, 65, 131, 142	0
1	B	496/496 (100%)	0.38	41 (8%) <b>11</b> <b>9</b>	28, 54, 103, 122	0
1	C	496/496 (100%)	0.92	95 (19%) <b>1</b> <b>0</b>	26, 50, 128, 153	0
1	D	496/496 (100%)	0.34	45 (9%) <b>9</b> <b>7</b>	25, 52, 109, 126	0
1	E	496/496 (100%)	-0.04	20 (4%) 38 37	27, 49, 84, 116	0
1	F	496/496 (100%)	0.44	65 (13%) <b>3</b> <b>2</b>	29, 54, 113, 133	0
All	All	2976/2976 (100%)	0.43	330 (11%) <b>5</b> <b>4</b>	25, 54, 116, 153	0

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	313	PRO	15.4
1	C	303	GLY	14.3
1	A	36	LEU	14.1
1	C	316	GLY	11.6
1	C	300	LEU	11.3
1	D	36	LEU	10.2
1	C	280	SER	10.1
1	C	314	TYR	9.5
1	C	10	ASP	8.7
1	D	309	PRO	8.6
1	C	317	SER	8.4
1	F	36	LEU	8.4
1	E	428	HIS	8.1
1	A	38	THR	8.1
1	C	281	ASP	8.0
1	C	296	GLU	7.9
1	A	317	SER	7.8
1	C	306	LEU	7.7
1	C	255	GLY	7.6

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Mol	Chain	Res	Type	RSRZ
1	F	505	THR	7.3
1	C	12	ASN	7.3
1	C	302	HIS	7.2
1	C	35	ASP	7.1
1	C	268	HIS	7.1
1	C	311	ALA	6.9
1	C	285	TRP	6.8
1	D	35	ASP	6.8
1	D	428	HIS	6.8
1	A	428	HIS	6.6
1	A	312	LYS	6.5
1	C	274	CYS	6.5
1	C	308	PHE	6.5
1	C	301	GLN	6.4
1	C	256	PHE	6.3
1	F	317	SER	6.2
1	C	11	PRO	6.1
1	D	38	THR	6.0
1	D	34	GLU	5.9
1	C	40	GLU	5.9
1	A	35	ASP	5.7
1	C	318	ILE	5.7
1	C	428	HIS	5.6
1	A	300	LEU	5.5
1	C	284	ILE	5.5
1	C	279	GLU	5.5
1	F	10	ASP	5.4
1	D	300	LEU	5.3
1	C	13	PHE	5.3
1	A	313	PRO	5.2
1	B	38	THR	5.2
1	C	254	GLN	5.1
1	A	306	LEU	5.1
1	B	35	ASP	5.0
1	A	309	PRO	5.0
1	A	338	SER	5.0
1	A	33	VAL	5.0
1	F	281	ASP	4.9
1	B	309	PRO	4.9
1	C	264	MET	4.9
1	A	311	ALA	4.8
1	C	253	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	295	LEU	4.7
1	C	288	ASP	4.6
1	A	316	GLY	4.6
1	C	290	ILE	4.6
1	F	35	ASP	4.6
1	A	298	PHE	4.5
1	B	428	HIS	4.5
1	B	298	PHE	4.5
1	B	13	PHE	4.5
1	E	38	THR	4.5
1	C	289	GLY	4.5
1	D	40	GLU	4.4
1	D	13	PHE	4.4
1	A	32	LEU	4.4
1	F	313	PRO	4.4
1	C	304	SER	4.4
1	A	505	THR	4.4
1	F	247	GLY	4.3
1	E	505	THR	4.3
1	D	10	ASP	4.3
1	B	342	ARG	4.3
1	C	298	PHE	4.3
1	D	338	SER	4.3
1	F	337	LYS	4.3
1	E	40	GLU	4.2
1	B	40	GLU	4.2
1	D	305	ILE	4.2
1	F	239	ILE	4.2
1	E	36	LEU	4.2
1	D	33	VAL	4.2
1	B	318	ILE	4.2
1	F	336	THR	4.2
1	C	261	LEU	4.1
1	A	280	SER	4.1
1	D	12	ASN	4.1
1	C	305	ILE	4.0
1	C	39	ARG	4.0
1	A	13	PHE	4.0
1	A	343	VAL	4.0
1	C	272	ALA	4.0
1	F	303	GLY	3.9
1	C	42	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	429	GLY	3.9
1	C	38	THR	3.9
1	C	277	VAL	3.9
1	A	37	ARG	3.9
1	A	369	ILE	3.9
1	D	337	LYS	3.8
1	F	11	PRO	3.8
1	A	270	PHE	3.8
1	B	36	LEU	3.8
1	D	342	ARG	3.7
1	A	349	ALA	3.7
1	F	316	GLY	3.7
1	D	505	THR	3.7
1	F	338	SER	3.7
1	E	35	ASP	3.7
1	F	314	TYR	3.6
1	E	39	ARG	3.6
1	A	285	TRP	3.6
1	A	341	PRO	3.6
1	C	326	LEU	3.6
1	B	429	GLY	3.6
1	B	305	ILE	3.6
1	F	280	SER	3.6
1	D	359	GLU	3.6
1	C	267	LEU	3.5
1	A	34	GLU	3.5
1	D	31	LYS	3.5
1	A	302	HIS	3.5
1	E	316	GLY	3.5
1	B	344	LYS	3.5
1	B	11	PRO	3.4
1	F	37	ARG	3.4
1	C	307	GLY	3.4
1	E	429	GLY	3.4
1	A	342	ARG	3.4
1	C	252	VAL	3.4
1	C	297	ASP	3.4
1	C	250	THR	3.4
1	F	252	VAL	3.4
1	C	275	ILE	3.4
1	E	503	THR	3.3
1	C	312	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	276	ALA	3.3
1	F	302	HIS	3.3
1	D	289	GLY	3.3
1	C	292	PRO	3.3
1	D	42	GLU	3.3
1	D	322	ASP	3.3
1	F	306	LEU	3.3
1	B	34	GLU	3.3
1	F	42	GLU	3.3
1	C	36	LEU	3.3
1	F	32	LEU	3.2
1	A	336	THR	3.2
1	C	247	GLY	3.2
1	F	285	TRP	3.2
1	F	284	ILE	3.2
1	C	293	LYS	3.2
1	C	433	PRO	3.2
1	A	41	SER	3.2
1	C	263	SER	3.2
1	A	366	GLU	3.1
1	F	38	THR	3.1
1	C	286	ASN	3.1
1	B	270	PHE	3.1
1	C	14	PHE	3.1
1	C	310	LYS	3.1
1	D	326	LEU	3.1
1	C	299	LYS	3.1
1	F	277	VAL	3.1
1	F	325	ILE	3.1
1	C	34	GLU	3.0
1	C	323	CYS	3.0
1	B	12	ASN	3.0
1	A	282	GLY	3.0
1	F	333	LYS	3.0
1	C	429	GLY	3.0
1	C	260	GLY	3.0
1	D	247	GLY	3.0
1	F	328	PRO	3.0
1	B	41	SER	3.0
1	D	11	PRO	3.0
1	B	432	ILE	2.9
1	F	12	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	359	GLU	2.9
1	B	43	GLU	2.9
1	C	331	SER	2.9
1	E	41	SER	2.9
1	D	297	ASP	2.9
1	F	254	GLN	2.9
1	D	293	LYS	2.9
1	B	278	GLY	2.9
1	C	251	PHE	2.9
1	C	336	THR	2.9
1	C	502	VAL	2.9
1	F	41	SER	2.9
1	D	315	GLU	2.9
1	A	12	ASN	2.9
1	C	337	LYS	2.8
1	A	327	ILE	2.8
1	A	308	PHE	2.8
1	A	429	GLY	2.8
1	D	314	TYR	2.8
1	B	297	ASP	2.8
1	C	319	LEU	2.8
1	C	309	PRO	2.8
1	D	301	GLN	2.8
1	A	427	LYS	2.7
1	D	251	PHE	2.7
1	E	13	PHE	2.7
1	B	264	MET	2.7
1	D	14	PHE	2.7
1	D	308	PHE	2.7
1	F	300	LEU	2.7
1	E	342	ARG	2.7
1	A	323	CYS	2.7
1	A	328	PRO	2.7
1	C	339	ASN	2.7
1	F	346	LYS	2.7
1	B	10	ASP	2.6
1	A	433	PRO	2.6
1	F	326	LEU	2.6
1	A	47	ASN	2.6
1	C	505	THR	2.6
1	B	338	SER	2.6
1	F	359	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	339	ASN	2.5
1	F	349	ALA	2.5
1	A	40	GLU	2.5
1	B	435	VAL	2.5
1	F	40	GLU	2.5
1	A	11	PRO	2.5
1	F	318	ILE	2.5
1	A	39	ARG	2.5
1	B	294	GLU	2.5
1	F	298	PHE	2.5
1	B	505	THR	2.5
1	C	243	THR	2.5
1	A	246	PHE	2.5
1	B	293	LYS	2.5
1	D	344	LYS	2.5
1	F	504	PHE	2.5
1	F	45	LYS	2.5
1	F	297	ASP	2.5
1	B	446	GLY	2.4
1	A	337	LYS	2.4
1	D	39	ARG	2.4
1	A	10	ASP	2.4
1	C	294	GLU	2.4
1	C	329	ALA	2.4
1	B	255	GLY	2.4
1	A	333	LYS	2.4
1	F	312	LYS	2.4
1	A	326	LEU	2.4
1	A	377	LEU	2.4
1	A	307	GLY	2.4
1	B	341	PRO	2.4
1	B	314	TYR	2.3
1	E	33	VAL	2.3
1	C	291	ASP	2.3
1	A	363	ILE	2.3
1	B	427	LYS	2.3
1	E	425	PHE	2.3
1	A	266	TYR	2.3
1	B	246	PHE	2.3
1	F	251	PHE	2.3
1	C	273	LYS	2.3
1	C	325	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	333	LYS	2.3
1	F	331	SER	2.3
1	F	373	PRO	2.3
1	C	356	THR	2.3
1	F	356	THR	2.3
1	F	372	ILE	2.3
1	B	474	LYS	2.3
1	B	289	GLY	2.2
1	F	335	LEU	2.2
1	F	39	ARG	2.2
1	F	253	VAL	2.2
1	F	354	GLY	2.2
1	C	240	LEU	2.2
1	F	309	PRO	2.2
1	F	341	PRO	2.2
1	D	250	THR	2.2
1	A	314	TYR	2.2
1	D	246	PHE	2.2
1	C	44	GLN	2.2
1	F	470	ARG	2.2
1	C	349	ALA	2.2
1	C	246	PHE	2.2
1	E	42	GLU	2.2
1	D	292	PRO	2.2
1	C	354	GLY	2.2
1	B	253	VAL	2.2
1	F	428	HIS	2.2
1	E	427	LYS	2.2
1	F	276	ALA	2.2
1	D	274	CYS	2.2
1	C	266	TYR	2.1
1	C	33	VAL	2.1
1	D	446	GLY	2.1
1	E	12	ASN	2.1
1	E	14	PHE	2.1
1	B	283	SER	2.1
1	A	354	GLY	2.1
1	E	34	GLU	2.1
1	B	247	GLY	2.1
1	C	15	LYS	2.1
1	D	339	ASN	2.1
1	C	504	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	44	GLN	2.1
1	F	48	ARG	2.1
1	A	14	PHE	2.1
1	A	255	GLY	2.1
1	A	288	ASP	2.1
1	A	351	GLY	2.1
1	D	43	GLU	2.1
1	A	42	GLU	2.1
1	A	43	GLU	2.1
1	D	269	ARG	2.0
1	F	274	CYS	2.0
1	C	242	MET	2.0
1	D	270	PHE	2.0
1	A	284	ILE	2.0
1	A	279	GLU	2.0
1	F	241	GLY	2.0
1	F	357	THR	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, 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( $\text{\AA}^2$ )	Q<0.9
2	PO4	B	601	5/5	0.74	0.28	75,87,101,103	0
2	PO4	A	1001	5/5	0.79	0.16	49,65,83,100	0
2	PO4	C	602	5/5	0.82	0.17	39,41,54,80	0
2	PO4	F	2003	5/5	0.82	0.19	49,60,69,91	0
2	PO4	D	601	5/5	0.87	0.35	58,60,88,89	0
2	PO4	F	2001	5/5	0.92	0.27	55,68,72,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	E	603	5/5	0.92	0.21	50,62,64,78	0
2	PO4	E	601	5/5	0.93	0.32	52,55,68,87	0
2	PO4	C	601	5/5	0.94	0.10	61,65,79,81	0
2	PO4	E	602	5/5	0.95	0.14	53,55,63,75	0
2	PO4	F	2002	5/5	0.95	0.12	55,64,70,76	0
2	PO4	B	602	5/5	0.95	0.09	71,74,81,94	0
2	PO4	D	602	5/5	0.96	0.21	68,69,74,91	0
2	PO4	F	2004	5/5	0.97	0.10	39,43,46,53	0
2	PO4	D	603	5/5	0.98	0.14	34,38,43,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.