



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:25 PM GMT

PDB ID : 4XRP  
Title : Structure of the Pnkp1/Rnl/Hen1 RNA repair complex  
Authors : Huang, R.H.; Wang, P.  
Deposited on : 2015-01-21  
Resolution : 3.30 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

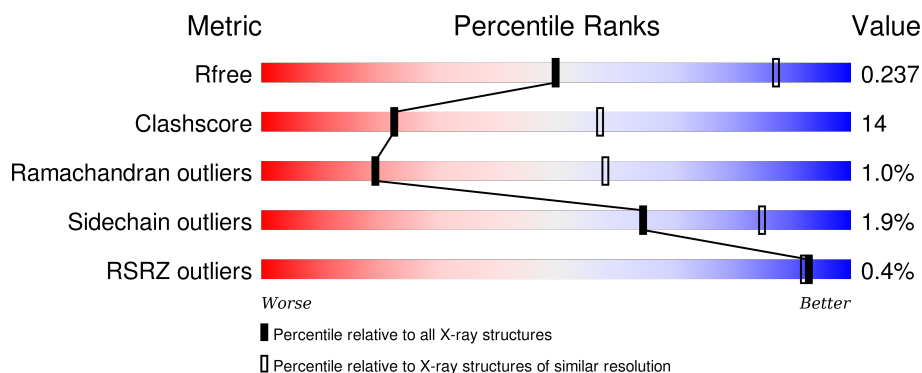
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	312	<div> <div>65%</div> <div>33%</div> <div>..</div> </div>
1	D	312	<div> <div>58%</div> <div>39%</div> <div>..</div> </div>
2	B	394	<div> <div>70%</div> <div>28%</div> <div>.</div> </div>
2	E	394	<div> <div>71%</div> <div>28%</div> <div>.</div> </div>
3	C	436	<div> <div>66%</div> <div>29%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	436	

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
4	PO4	A	401	-	-	X	-
5	MG	A	402	-	-	-	X
5	MG	D	402	-	-	-	X
6	SO4	A	403	-	-	-	X
6	SO4	C	501	-	-	-	X
6	SO4	E	401	-	-	-	X
6	SO4	F	502	-	-	-	X
7	GOL	B	404	-	-	-	X
7	GOL	C	503	-	-	-	X
7	GOL	C	504	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18888 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 Pnkp1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2544	1620	433	479	12			
1	D	311	Total	C	N	O	S	0	0	0
			2544	1620	433	479	12			

- Molecule 2 is a protein called Rnl.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	0	0
			3289	2116	557	607	9			
2	E	393	Total	C	N	O	S	0	0	0
			3281	2111	556	606	8			

- Molecule 3 is a protein called Hen1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	424	Total	C	N	O	S	0	0	0
			3537	2286	580	654	17			
3	F	422	Total	C	N	O	S	0	0	0
			3516	2271	576	652	17			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

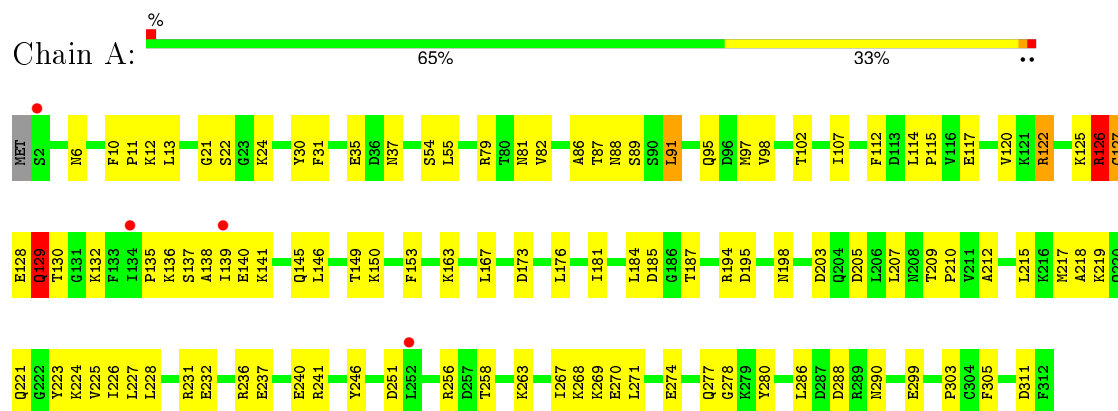
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total	O	0	0
			7	7		
8	B	18	Total	O	0	0
			18	18		
8	C	22	Total	O	0	0
			22	22		
8	D	9	Total	O	0	0
			9	9		
8	E	17	Total	O	0	0
			17	17		
8	F	20	Total	O	0	0
			20	20		

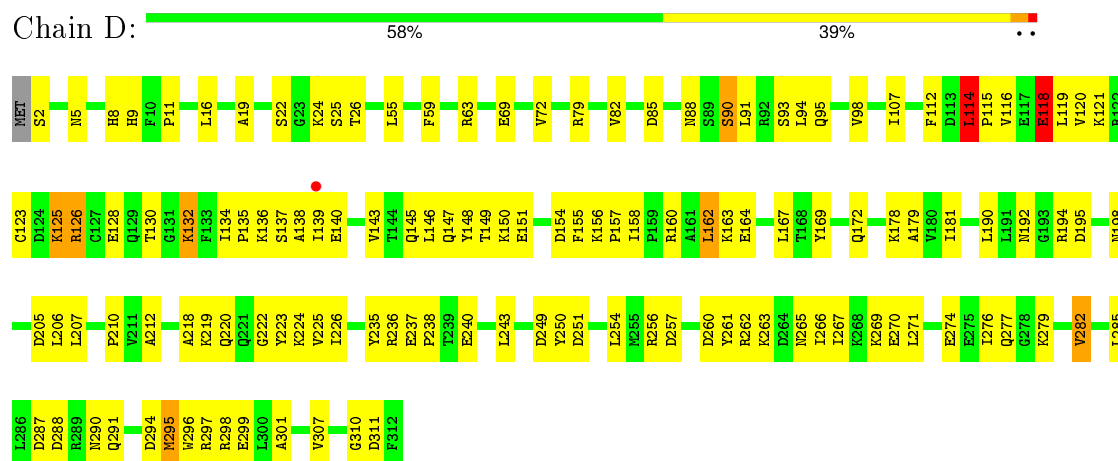
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

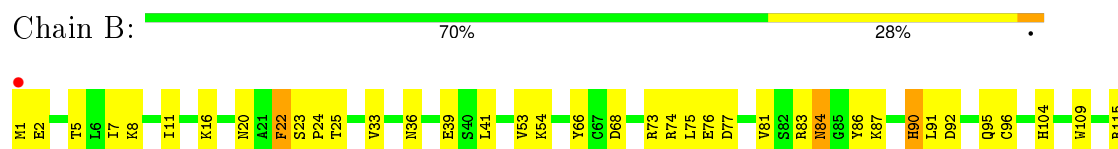
#### • Molecule 1: Pnkp1



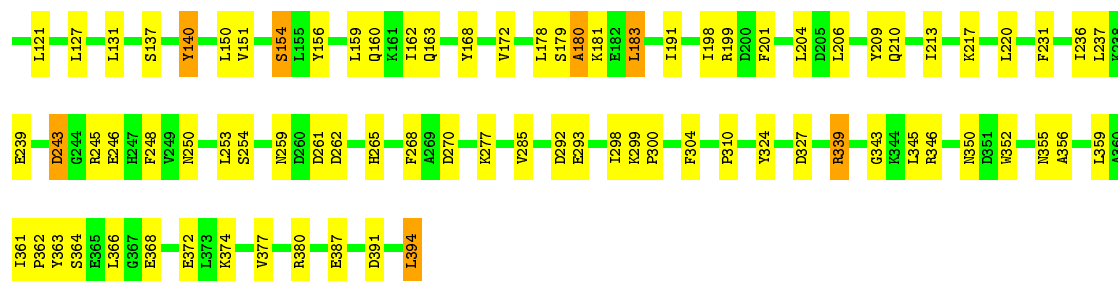
#### • Molecule 1: Pnkp1



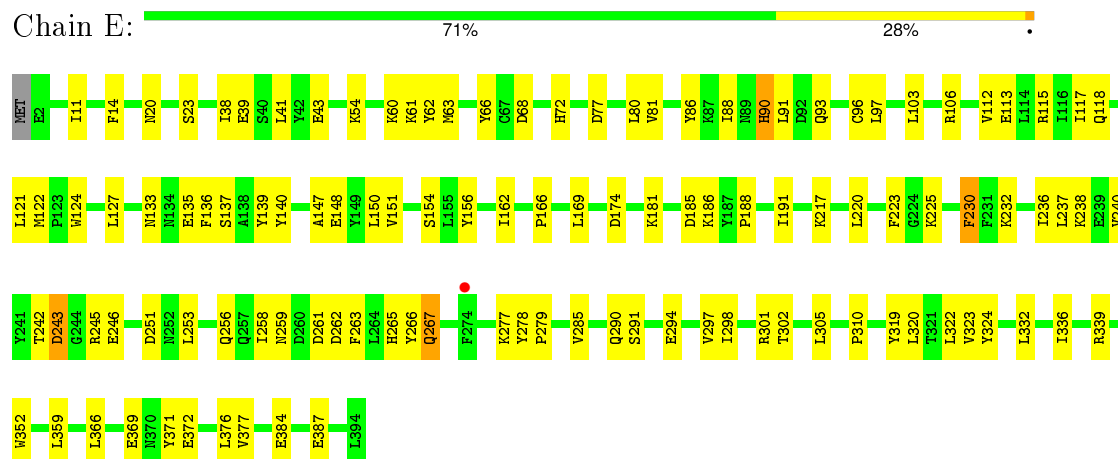
#### • Molecule 2: Rnl



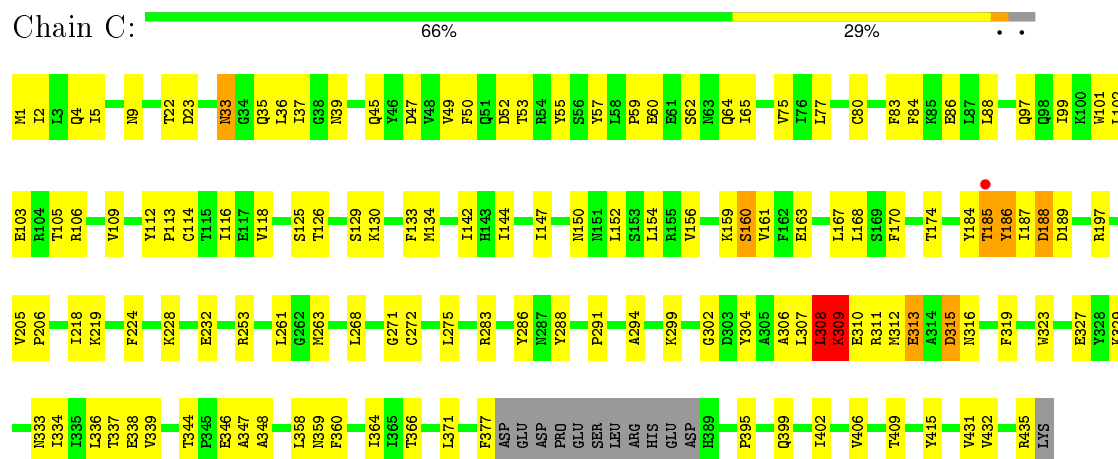




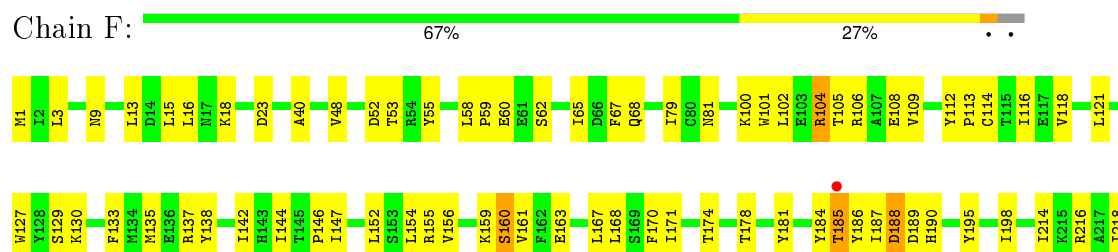
• Molecule 2: Rnl

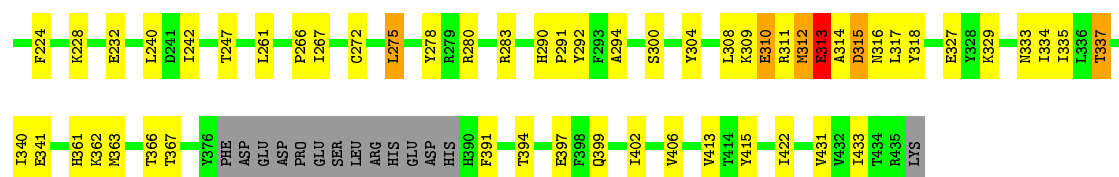


• Molecule 3: Hen1



• Molecule 3: Hen1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.16Å 179.20Å 114.33Å 90.00° 103.70° 90.00°	Depositor
Resolution (Å)	47.21 – 3.30 47.21 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.21-3.30) 96.7 (47.21-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.02 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1624)	Depositor
R, $R_{free}$	0.175 , 0.238 0.176 , 0.237	Depositor DCC
$R_{free}$ test set	1917 reflections (3.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.0	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.8	EDS
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 65456 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, PO4, SO4

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	0.52	2/2594 (0.1%)	0.81	3/3501 (0.1%)
1	D	0.52	0/2594	0.86	5/3501 (0.1%)
2	B	0.59	0/3366	0.78	3/4544 (0.1%)
2	E	0.52	0/3358	0.71	0/4534
3	C	0.57	0/3636	0.78	3/4932 (0.1%)
3	F	0.58	0/3613	0.76	2/4901 (0.0%)
All	All	0.56	2/19161 (0.0%)	0.78	16/25913 (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	D	0	1
3	C	0	2
3	F	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	GLN	CG-CD	6.51	1.66	1.51
1	A	129	GLN	CB-CG	5.11	1.66	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	309	LYS	CD-CE-NZ	7.75	129.52	111.70
1	D	126	ARG	CG-CD-NE	7.21	126.94	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	LEU	CA-CB-CG	6.80	130.95	115.30
2	B	183	LEU	CA-CB-CG	6.73	130.78	115.30
1	A	126	ARG	N-CA-C	-6.58	93.23	111.00
2	B	299	LYS	CD-CE-NZ	6.56	126.78	111.70
1	D	114	LEU	CA-CB-CG	6.54	130.35	115.30
3	C	308	LEU	CA-CB-CG	6.40	130.01	115.30
1	A	129	GLN	N-CA-C	6.25	127.87	111.00
2	B	394	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	129	GLN	N-CA-CB	-5.57	100.58	110.60
1	D	118	GLU	CA-CB-CG	5.56	125.63	113.40
3	C	33	ASN	N-CA-C	5.35	125.45	111.00
3	F	310	GLU	N-CA-C	-5.25	96.82	111.00
1	D	295	MET	CA-CB-CG	5.12	122.00	113.30
3	F	275	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	308	LEU	Peptide
3	C	64	GLN	Peptide
1	D	118	GLU	Peptide
3	F	312	MET	Peptide
3	F	313	GLU	Peptide

## 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	2544	0	2543	79	0
1	D	2544	0	2543	100	0
2	B	3289	0	3251	76	0
2	E	3281	0	3239	82	0
3	C	3537	0	3404	93	0
3	F	3516	0	3388	101	0
4	A	5	0	0	2	0
4	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	D	1	0	0	0	0
6	A	10	0	0	0	0
6	B	5	0	0	1	0
6	C	5	0	0	0	0
6	E	10	0	0	0	0
6	F	10	0	0	0	0
7	B	6	0	8	1	0
7	C	18	0	24	2	0
7	F	6	0	8	2	0
8	A	7	0	0	0	0
8	B	18	0	0	3	0
8	C	22	0	0	2	0
8	D	9	0	0	0	0
8	E	17	0	0	4	0
8	F	20	0	0	4	0
All	All	18888	0	18408	508	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 14.

All (508) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ASN:HB2	2:B:366:LEU:HD11	1.34	1.06
1:A:126:ARG:O	1:A:128:GLU:N	1.96	0.98
3:F:160:SER:HB2	3:F:163:GLU:H	1.33	0.94
2:E:20:ASN:HB2	2:E:366:LEU:HD11	1.50	0.91
1:D:5:ASN:ND2	3:F:318:TYR:OH	2.05	0.89
3:F:100:LYS:HA	3:F:102:LEU:H	1.39	0.87
3:F:216:ARG:NH1	7:F:503:GOL:O2	2.08	0.86
2:B:324:TYR:OH	2:B:339:ARG:NH1	2.09	0.86
3:C:156:VAL:HG13	3:C:167:LEU:HD23	1.56	0.86
3:C:160:SER:HB2	3:C:163:GLU:H	1.40	0.85
1:A:129:GLN:CD	1:A:130:THR:H	1.81	0.83
1:D:172:GLN:HE22	1:D:282:VAL:HG23	1.44	0.82
1:A:203:ASP:OD2	1:A:241:ARG:NH2	2.12	0.82
1:A:269:LYS:NZ	1:A:299:GLU:OE1	2.13	0.82
3:C:337:THR:HA	3:C:366:THR:HB	1.60	0.81
3:F:100:LYS:HG2	3:F:101:TRP:HA	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:9:ASN:HB2	3:F:112:TYR:HB2	1.64	0.80
2:E:140:TYR:CE2	2:E:217:LYS:HG3	2.17	0.79
1:A:221:GLN:NE2	1:D:220:GLN:OE1	2.15	0.79
3:C:308:LEU:HB3	3:C:313:GLU:HB3	1.65	0.79
3:C:308:LEU:N	3:C:309:LYS:HB3	1.99	0.78
3:F:242:ILE:HD12	3:F:422:ILE:HG12	1.67	0.77
1:A:138:ALA:HA	1:A:141:LYS:HD2	1.66	0.77
2:E:41:LEU:HD22	2:E:285:VAL:HG21	1.67	0.76
3:C:308:LEU:H	3:C:309:LYS:HB3	1.48	0.76
1:A:217:MET:HE1	1:D:218:ALA:HA	1.68	0.75
3:F:216:ARG:HH12	7:F:503:GOL:HO2	1.35	0.75
2:B:39:GLU:HG2	2:B:339:ARG:HH21	1.51	0.74
2:E:140:TYR:CZ	2:E:217:LYS:HG3	2.23	0.74
1:D:88:ASN:HB3	1:D:93:SER:OG	1.88	0.73
2:E:225:LYS:O	8:E:516:HOH:O	2.07	0.73
2:B:137:SER:HB3	2:B:220:LEU:HD21	1.71	0.73
1:D:218:ALA:O	1:D:223:TYR:HB2	1.89	0.72
1:D:118:GLU:HB2	1:D:121:LYS:HB3	1.71	0.71
2:E:243:ASP:OD2	2:E:245:ARG:NH1	2.23	0.71
2:E:80:LEU:HB2	2:E:88:ILE:HB	1.70	0.71
1:D:167:LEU:HD21	1:D:169:TYR:CZ	2.25	0.71
1:D:192:ASN:HD22	1:D:206:LEU:HD12	1.56	0.71
1:A:126:ARG:HG2	1:A:129:GLN:HG3	1.73	0.70
3:C:291:PRO:HA	3:C:316:ASN:HB2	1.73	0.69
1:D:224:LYS:HD2	1:D:251:ASP:OD2	1.92	0.69
2:E:68:ASP:HB2	2:E:81:VAL:HG13	1.75	0.69
2:B:2:GLU:OE2	8:B:503:HOH:O	2.12	0.68
3:F:267:ILE:HD11	3:F:292:TYR:CZ	2.28	0.68
3:F:156:VAL:HG13	3:F:167:LEU:HD23	1.74	0.68
3:C:261:LEU:HD22	3:C:333:ASN:HB3	1.76	0.67
3:C:116:ILE:HG21	3:C:168:LEU:HD22	1.76	0.67
3:C:344:THR:HG22	3:C:347:ALA:H	1.59	0.67
3:F:283:ARG:HH11	3:F:283:ARG:CG	2.08	0.66
2:E:93:GLN:O	2:E:97:LEU:HG	1.96	0.65
3:F:106:ARG:NH1	8:F:612:HOH:O	2.28	0.65
2:E:139:TYR:CD2	3:F:65:ILE:HG22	2.32	0.65
1:D:226:ILE:HG21	1:D:276:ILE:HD11	1.79	0.65
1:A:86:ALA:HA	1:A:97:MET:HE1	1.80	0.64
1:A:187:THR:OG1	1:A:288:ASP:HB3	1.97	0.64
1:A:21:GLY:HA2	1:A:126:ARG:HH21	1.63	0.64
1:D:194:ARG:NH1	1:D:205:ASP:OD2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:340:ILE:HD11	3:F:367:THR:HB	1.80	0.64
1:D:72:VAL:HG13	1:D:82:VAL:HG11	1.79	0.64
3:C:253:ARG:HD3	3:C:366:THR:HG21	1.79	0.64
2:E:232:LYS:NZ	2:E:261:ASP:OD2	2.21	0.64
2:E:181:LYS:NZ	2:E:185:ASP:OD2	2.31	0.63
3:F:267:ILE:HD11	3:F:292:TYR:CE2	2.32	0.63
3:F:309:LYS:NZ	3:F:314:ALA:HB2	2.13	0.63
3:F:240:LEU:HB3	3:F:242:ILE:HD11	1.79	0.63
3:C:129:SER:HA	7:C:503:GOL:H11	1.81	0.63
2:B:41:LEU:HD22	2:B:285:VAL:HG21	1.81	0.63
1:D:119:LEU:HB3	1:D:139:ILE:HD11	1.81	0.63
1:A:185:ASP:OD1	1:A:231:ARG:NE	2.31	0.63
1:D:192:ASN:HD22	1:D:206:LEU:CD1	2.12	0.62
1:D:79:ARG:HD2	3:F:311:ARG:HE	1.64	0.62
3:C:310:GLU:HG2	3:C:312:MET:HB2	1.81	0.62
1:D:98:VAL:HG13	1:D:107:ILE:HD12	1.81	0.61
1:A:117:GLU:HA	1:A:120:VAL:HG22	1.81	0.61
1:A:141:LYS:O	1:A:145:GLN:HB2	1.99	0.61
3:C:188:ASP:OD1	3:C:189:ASP:N	2.33	0.61
2:E:63:MET:HG2	2:E:124:TRP:CD1	2.36	0.61
1:A:6:ASN:HB3	1:D:261:TYR:CE1	2.36	0.61
3:F:186:TYR:HD1	3:F:188:ASP:H	1.47	0.60
3:F:214:ILE:HA	3:F:218:ILE:HD13	1.83	0.60
2:E:240:VAL:HG22	2:E:246:GLU:HG2	1.82	0.60
2:B:68:ASP:HB2	2:B:81:VAL:HG23	1.82	0.60
3:F:59:PRO:HG2	3:F:184:TYR:HB3	1.83	0.60
2:B:179:SER:O	2:B:181:LYS:N	2.33	0.60
1:A:218:ALA:O	1:A:223:TYR:HB2	2.01	0.60
1:A:24:LYS:HB2	4:A:401:PO4:O1	2.01	0.60
1:A:237:GLU:O	1:A:241:ARG:HD3	2.01	0.59
2:E:61:LYS:HB2	2:E:297:VAL:HG23	1.84	0.59
2:E:148:GLU:HG2	8:E:515:HOH:O	2.02	0.59
1:A:194:ARG:NH1	1:A:205:ASP:OD2	2.36	0.59
1:D:16:LEU:HB2	1:D:85:ASP:HA	1.85	0.59
2:E:232:LYS:HE3	2:E:259:ASN:HD21	1.67	0.59
2:E:113:GLU:HG3	2:E:242:THR:HG22	1.85	0.59
1:A:129:GLN:NE2	1:A:130:THR:OG1	2.36	0.59
1:D:172:GLN:NE2	1:D:282:VAL:HG23	2.14	0.59
1:D:256:ARG:HG3	1:D:267:ILE:HD13	1.84	0.59
3:C:59:PRO:HG2	3:C:184:TYR:HB3	1.85	0.59
2:E:39:GLU:HG2	2:E:339:ARG:HH12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HB3	1:D:190:LEU:HD21	1.85	0.58
3:C:327:GLU:O	3:C:329:LYS:HG2	2.02	0.58
2:E:23:SER:HB3	2:E:66:TYR:CE1	2.39	0.58
3:C:271:GLY:HA3	3:C:339:VAL:HG11	1.84	0.58
1:D:130:THR:OG1	1:D:132:LYS:NZ	2.18	0.58
2:E:290:GLN:HG3	2:E:291:SER:N	2.19	0.58
3:F:144:ILE:HD12	3:F:152:LEU:HD13	1.85	0.58
3:F:283:ARG:HH11	3:F:283:ARG:HG2	1.69	0.57
1:A:120:VAL:HG11	1:A:136:LYS:HD3	1.85	0.57
1:A:277:GLN:HG3	1:A:278:GLY:N	2.19	0.57
3:C:9:ASN:HB2	3:C:112:TYR:HB2	1.85	0.57
1:D:145:GLN:O	1:D:149:THR:HG23	2.03	0.57
3:F:341:GLU:HA	3:F:391:PHE:CE2	2.39	0.57
1:D:135:PRO:C	1:D:137:SER:H	2.06	0.57
3:C:105:THR:O	3:C:109:VAL:HG23	2.04	0.57
3:F:413:VAL:HG22	3:F:433:ILE:HG12	1.86	0.57
3:C:129:SER:OG	3:C:130:LYS:N	2.38	0.57
1:D:136:LYS:HA	1:D:139:ILE:HG22	1.85	0.57
2:B:41:LEU:HD12	2:B:298:ILE:HD11	1.85	0.57
1:A:135:PRO:HG2	1:A:138:ALA:H	1.69	0.57
2:B:162:ILE:HD12	3:C:23:ASP:HB3	1.87	0.57
1:D:118:GLU:HA	1:D:121:LYS:H	1.68	0.57
3:F:52:ASP:OD1	3:F:53:THR:N	2.38	0.57
1:A:146:LEU:HD21	1:A:150:LYS:HD2	1.87	0.57
1:A:129:GLN:HG2	1:A:130:THR:HG23	1.86	0.56
2:B:39:GLU:CG	2:B:339:ARG:HH21	2.18	0.56
1:A:184:LEU:HD11	1:A:227:LEU:HD23	1.87	0.56
3:F:62:SER:HB3	3:F:184:TYR:CD2	2.40	0.56
3:C:268:LEU:HD23	3:C:334:ILE:HD12	1.86	0.56
1:D:154:ASP:OD1	1:D:156:LYS:HG2	2.04	0.56
1:D:91:LEU:HB2	1:D:149:THR:CG2	2.36	0.56
3:C:147:ILE:HG13	3:C:152:LEU:HA	1.86	0.56
3:F:114:CYS:SG	3:F:161:VAL:HG22	2.46	0.56
2:E:93:GLN:NE2	8:E:514:HOH:O	2.18	0.56
3:F:188:ASP:OD1	3:F:189:ASP:N	2.38	0.56
3:F:312:MET:O	3:F:313:GLU:HG2	2.06	0.56
3:F:104:ARG:HG3	3:F:108:GLU:CD	2.26	0.56
1:A:195:ASP:HB3	1:A:198:ASN:HB3	1.88	0.56
1:D:254:LEU:HB3	1:D:271:LEU:HD22	1.88	0.56
3:C:99:ILE:HD12	3:C:109:VAL:HG21	1.86	0.55
2:B:140:TYR:OH	2:B:217:LYS:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:267:ILE:HD13	3:F:335:ILE:HD12	1.88	0.55
1:D:114:LEU:HB2	1:D:115:PRO:HD2	1.88	0.55
2:E:112:VAL:HG11	2:E:115:ARG:CZ	2.36	0.55
3:C:364:ILE:HG12	3:C:432:VAL:HG22	1.88	0.55
1:D:25:SER:OG	1:D:26:THR:N	2.40	0.55
2:E:236:ILE:HD11	2:E:258:ILE:HD12	1.87	0.55
1:A:114:LEU:HD11	1:A:122:ARG:NH2	2.21	0.55
3:F:105:THR:O	3:F:109:VAL:HG23	2.06	0.55
1:D:235:TYR:C	1:D:238:PRO:HD2	2.27	0.55
3:C:263:MET:HE3	3:C:288:TYR:HD1	1.71	0.55
2:B:1:MET:HE3	2:B:7:ILE:HG12	1.89	0.55
2:E:369:GLU:HG2	2:E:371:TYR:HE2	1.71	0.55
2:E:162:ILE:HD13	3:F:23:ASP:HB3	1.87	0.55
3:F:187:ILE:HG22	3:F:187:ILE:O	2.07	0.55
1:D:269:LYS:NZ	1:D:299:GLU:OE1	2.40	0.54
3:C:307:LEU:HA	3:C:309:LYS:HG2	1.88	0.54
1:D:16:LEU:HD22	1:D:112:PHE:HE1	1.72	0.54
1:D:94:LEU:HD21	1:D:155:PHE:HE1	1.72	0.54
1:D:181:ILE:HD11	1:D:276:ILE:HD13	1.89	0.54
3:C:371:LEU:HG	3:C:395:PRO:HD2	1.88	0.54
2:E:121:LEU:HD23	2:E:127:LEU:HD22	1.90	0.54
3:F:309:LYS:HZ3	3:F:314:ALA:HB2	1.72	0.54
1:D:290:ASN:HB2	1:D:311:ASP:H	1.73	0.54
3:C:118:VAL:HB	3:C:154:LEU:HB3	1.89	0.54
3:C:313:GLU:O	3:C:315:ASP:HB3	2.08	0.54
1:D:22:SER:HA	1:D:114:LEU:HD11	1.90	0.54
3:C:299:LYS:HG3	3:C:302:GLY:HA3	1.90	0.54
3:F:13:LEU:HD21	3:F:40:ALA:HB1	1.89	0.54
2:E:302:THR:HB	2:E:305:LEU:HD11	1.90	0.54
2:B:74:ARG:HG2	2:B:76:GLU:HG2	1.89	0.54
1:D:207:LEU:HD11	1:D:212:ALA:HB2	1.90	0.54
3:F:147:ILE:HG13	3:F:152:LEU:HA	1.89	0.53
2:E:237:LEU:HD13	2:E:359:LEU:HD11	1.90	0.53
3:F:1:MET:HE1	3:F:118:VAL:HG13	1.89	0.53
2:E:251:ASP:OD1	2:E:253:LEU:HB2	2.08	0.53
1:A:91:LEU:H	1:A:149:THR:HG21	1.73	0.53
2:B:68:ASP:HB2	2:B:81:VAL:CG2	2.38	0.53
2:E:147:ALA:O	2:E:151:VAL:HG22	2.08	0.53
3:C:308:LEU:O	3:C:313:GLU:HB3	2.08	0.53
1:A:22:SER:HA	1:A:114:LEU:HD12	1.90	0.53
1:D:128:GLU:OE1	1:D:128:GLU:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ARG:HD2	3:F:311:ARG:NE	2.23	0.53
3:F:337:THR:HA	3:F:366:THR:HB	1.91	0.53
1:D:19:ALA:O	1:D:22:SER:OG	2.19	0.53
3:F:62:SER:HB3	3:F:184:TYR:HD2	1.74	0.53
1:D:8:HIS:C	1:D:9:HIS:HD2	2.12	0.53
1:D:126:ARG:HD2	1:D:132:LYS:NZ	2.24	0.53
1:D:90:SER:C	1:D:149:THR:HG21	2.29	0.52
2:E:323:VAL:O	3:F:65:ILE:HD11	2.09	0.52
2:B:361:ILE:HD11	2:B:372:GLU:HG2	1.91	0.52
2:B:204:LEU:HD21	8:C:609:HOH:O	2.09	0.52
3:F:129:SER:OG	3:F:130:LYS:N	2.41	0.52
1:A:91:LEU:O	1:A:95:GLN:HG3	2.09	0.52
1:D:88:ASN:OD1	1:D:90:SER:HB3	2.10	0.52
3:C:125:SER:OG	3:C:126:THR:N	2.39	0.52
1:A:207:LEU:HD11	1:A:212:ALA:HB2	1.92	0.52
1:A:232:GLU:HG2	1:A:258:THR:HA	1.92	0.52
2:B:91:LEU:HD23	2:B:92:ASP:N	2.26	0.51
1:A:11:PRO:HG3	1:A:79:ARG:HA	1.92	0.51
1:D:91:LEU:HB2	1:D:149:THR:HG22	1.91	0.51
3:C:344:THR:HG22	3:C:346:GLU:N	2.26	0.51
2:E:43:GLU:OE2	8:E:509:HOH:O	2.18	0.51
1:A:267:ILE:HD12	1:A:271:LEU:HD12	1.92	0.51
3:F:394:THR:HG23	3:F:397:GLU:OE1	2.10	0.51
2:B:115:ARG:HG2	2:B:239:GLU:HG2	1.92	0.51
3:C:55:TYR:CZ	3:C:60:GLU:HG3	2.46	0.51
1:A:31:PHE:CE1	1:A:35:GLU:HG3	2.46	0.51
1:D:160:ARG:HH22	1:D:162:LEU:HD22	1.76	0.51
1:A:140:GLU:O	1:A:140:GLU:HG3	2.10	0.51
1:D:22:SER:HB2	1:D:112:PHE:HB3	1.93	0.51
1:D:125:LYS:O	1:D:125:LYS:HG3	2.11	0.51
1:A:145:GLN:O	1:A:149:THR:HG23	2.11	0.51
2:B:91:LEU:HD22	2:B:96:CYS:SG	2.51	0.51
1:D:116:VAL:O	1:D:120:VAL:HG23	2.10	0.51
1:A:88:ASN:CG	1:A:89:SER:H	2.14	0.51
1:A:228:LEU:HD22	1:A:268:LYS:HG2	1.93	0.51
1:D:90:SER:HA	1:D:145:GLN:HG2	1.91	0.51
1:A:256:ARG:HG3	1:A:267:ILE:HD13	1.93	0.51
2:B:277:LYS:NZ	8:B:510:HOH:O	2.42	0.51
1:A:226:ILE:HD11	1:A:280:TYR:CZ	2.46	0.51
2:B:84:ASN:HB2	2:B:86:TYR:CD2	2.46	0.51
3:C:338:GLU:HG2	3:C:366:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:VAL:HG13	2:B:199:ARG:HD3	1.93	0.51
3:F:266:PRO:HB3	3:F:290:HIS:HB3	1.93	0.51
2:B:237:LEU:HD13	2:B:359:LEU:HD11	1.91	0.50
2:B:236:ILE:HD12	2:B:254:SER:HB2	1.92	0.50
3:F:291:PRO:HA	3:F:316:ASN:HB2	1.92	0.50
1:D:294:ASP:OD1	1:D:298:ARG:NH1	2.35	0.50
3:F:283:ARG:NH1	3:F:283:ARG:CG	2.70	0.50
2:B:156:TYR:O	2:B:160:GLN:HG3	2.12	0.50
3:C:33:ASN:O	3:C:53:THR:OG1	2.21	0.50
2:E:188:PRO:HG2	2:E:191:ILE:HG12	1.92	0.50
3:F:100:LYS:HA	3:F:102:LEU:N	2.18	0.50
2:E:136:PHE:HE1	2:E:220:LEU:HD11	1.77	0.50
2:B:154:SER:HB2	3:C:39:ASN:HD21	1.77	0.50
3:C:313:GLU:CD	3:C:315:ASP:HA	2.32	0.50
2:E:266:TYR:HE2	2:E:277:LYS:HD3	1.76	0.50
2:B:11:ILE:HG12	2:B:377:VAL:HG11	1.93	0.50
2:E:262:ASP:OD1	2:E:263:PHE:N	2.45	0.50
3:F:399:GLN:HG2	3:F:415:TYR:CE2	2.47	0.49
2:E:103:LEU:HD11	2:E:258:ILE:HD11	1.95	0.49
2:E:103:LEU:HA	2:E:106:ARG:HD2	1.94	0.49
2:E:372:GLU:O	2:E:376:LEU:HD23	2.12	0.49
2:B:253:LEU:HD11	2:B:265:HIS:CE1	2.47	0.49
3:F:1:MET:HA	3:F:1:MET:HE3	1.95	0.49
1:D:236:ARG:O	1:D:240:GLU:HG2	2.12	0.49
3:C:275:LEU:HA	8:C:619:HOH:O	2.12	0.49
2:B:201:PHE:HA	3:C:35:GLN:HG3	1.93	0.49
1:A:98:VAL:O	1:A:102:THR:HB	2.13	0.49
3:F:283:ARG:NH2	8:F:605:HOH:O	2.45	0.49
2:B:150:LEU:HD13	2:B:156:TYR:CE2	2.47	0.49
3:F:116:ILE:HG21	3:F:168:LEU:HD22	1.94	0.49
2:E:369:GLU:HG2	2:E:371:TYR:CE2	2.48	0.49
1:D:219:LYS:HZ1	1:D:249:ASP:C	2.16	0.49
2:E:60:LYS:HE3	2:E:62:TYR:OH	2.13	0.49
1:D:287:ASP:OD1	1:D:288:ASP:N	2.39	0.49
2:B:16:LYS:HE3	2:B:368:GLU:OE1	2.13	0.49
2:B:259:ASN:OD1	2:B:261:ASP:HB2	2.12	0.49
2:E:41:LEU:HD12	2:E:298:ILE:HD11	1.95	0.49
2:E:14:PHE:CD2	2:E:377:VAL:HG21	2.48	0.49
2:B:33:VAL:N	6:B:403:SO4:O2	2.47	0.48
1:A:129:GLN:CG	1:A:130:THR:H	2.26	0.48
1:D:219:LYS:HE2	1:D:225:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:327:GLU:O	3:F:329:LYS:HG2	2.13	0.48
2:B:180:ALA:HA	2:B:183:LEU:HG	1.94	0.48
2:E:319:TYR:HA	2:E:322:LEU:HD12	1.96	0.48
1:D:143:VAL:O	1:D:147:GLN:HG2	2.13	0.48
2:E:38:ILE:HG12	2:E:339:ARG:CZ	2.43	0.48
1:D:178:LYS:HE3	1:D:222:GLY:HA3	1.96	0.48
1:D:121:LYS:HG3	1:D:121:LYS:O	2.13	0.48
3:F:133:PHE:HB2	3:F:144:ILE:HG13	1.96	0.48
1:D:297:ARG:O	1:D:301:ALA:HA	2.14	0.48
2:E:133:ASN:ND2	2:E:135:GLU:HB2	2.28	0.48
3:C:360:PHE:O	3:C:435:ARG:HD2	2.14	0.48
3:C:306:ALA:O	3:C:309:LYS:HE2	2.14	0.47
3:C:323:TRP:CZ3	3:C:358:LEU:HD11	2.48	0.47
2:E:88:ILE:HD12	2:E:127:LEU:HD11	1.95	0.47
1:D:11:PRO:HG3	1:D:79:ARG:HA	1.97	0.47
3:F:313:GLU:C	3:F:315:ASP:HB2	2.35	0.47
2:B:5:THR:HA	2:B:8:LYS:HE2	1.96	0.47
3:F:127:TRP:CE3	3:F:178:THR:HG21	2.49	0.47
3:C:359:ASN:HA	3:C:435:ARG:HH12	1.79	0.47
2:E:332:LEU:O	2:E:336:ILE:HG13	2.13	0.47
2:E:174:ASP:OD2	2:E:186:LYS:HE2	2.13	0.47
1:D:79:ARG:HD2	3:F:311:ARG:CD	2.45	0.47
2:E:166:PRO:HA	2:E:169:LEU:HB2	1.96	0.47
1:D:285:LEU:HD22	1:D:296:TRP:CD2	2.50	0.47
2:E:81:VAL:HA	2:E:86:TYR:O	2.15	0.47
1:A:207:LEU:HD22	1:A:246:TYR:HD2	1.79	0.47
3:C:97:GLN:NE2	3:C:106:ARG:HH11	2.12	0.47
2:B:304:PHE:CD2	2:B:356:ALA:HB2	2.50	0.47
2:B:73:ARG:HA	2:B:109:TRP:CE3	2.49	0.47
3:C:129:SER:C	3:C:130:LYS:HD3	2.35	0.47
2:E:294:GLU:HG2	2:E:319:TYR:CZ	2.48	0.47
2:B:310:PRO:HB3	2:B:352:TRP:CD2	2.49	0.47
1:D:146:LEU:O	1:D:150:LYS:N	2.43	0.47
3:F:272:CYS:SG	3:F:294:ALA:HB1	2.55	0.47
1:D:270:GLU:O	1:D:274:GLU:HG3	2.14	0.47
2:B:209:TYR:O	2:B:213:ILE:HG13	2.15	0.47
1:A:286:LEU:HD23	1:A:305:PHE:HB2	1.96	0.47
3:F:310:GLU:HG2	3:F:312:MET:HB2	1.97	0.46
3:C:218:ILE:HG21	3:C:224:PHE:HB2	1.97	0.46
3:F:113:PRO:HA	3:F:159:LYS:O	2.16	0.46
1:D:91:LEU:O	1:D:95:GLN:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:PRO:C	1:D:137:SER:N	2.69	0.46
1:A:146:LEU:O	1:A:150:LYS:N	2.47	0.46
3:C:399:GLN:HG2	3:C:415:TYR:CE2	2.51	0.46
1:A:263:LYS:HE2	1:A:263:LYS:HB3	1.75	0.46
3:F:170:PHE:HD2	3:F:171:ILE:HD13	1.80	0.46
3:C:57:TYR:CZ	3:C:75:VAL:HG22	2.50	0.46
2:B:350:ASN:HB3	8:B:516:HOH:O	2.16	0.46
3:F:1:MET:CE	3:F:118:VAL:HG13	2.45	0.46
1:A:98:VAL:HG13	1:A:107:ILE:HD12	1.97	0.46
2:B:66:TYR:CD2	7:B:404:GOL:H31	2.51	0.46
2:E:124:TRP:CH2	2:E:223:PHE:HB2	2.51	0.46
1:D:257:ASP:O	1:D:260:ASP:HB2	2.16	0.46
1:D:290:ASN:H	1:D:310:GLY:HA3	1.80	0.45
2:B:92:ASP:OD2	2:B:95:GLN:HB2	2.16	0.45
1:A:173:ASP:HB3	1:A:176:LEU:HD12	1.98	0.45
2:E:122:MET:HB2	2:E:230:PHE:CD2	2.51	0.45
3:C:88:LEU:O	3:C:197:ARG:NH2	2.31	0.45
2:B:53:VAL:HG11	2:B:300:PRO:HB3	1.99	0.45
1:A:290:ASN:HB2	1:A:311:ASP:H	1.81	0.45
2:E:320:LEU:HA	2:E:323:VAL:HG22	1.97	0.45
1:D:240:GLU:HA	1:D:243:LEU:HB2	1.99	0.45
3:F:170:PHE:O	3:F:174:THR:HG23	2.17	0.45
2:B:248:PHE:CD1	2:B:250:ASN:HB2	2.51	0.45
3:C:187:ILE:O	3:C:219:LYS:HE3	2.16	0.45
2:E:11:ILE:HG12	2:E:377:VAL:CG1	2.47	0.45
2:B:11:ILE:HG12	2:B:377:VAL:CG1	2.47	0.45
2:E:150:LEU:HD13	2:E:156:TYR:CE1	2.52	0.45
2:B:151:VAL:HG12	2:B:206:LEU:HD13	1.99	0.45
3:C:52:ASP:OD1	3:C:53:THR:N	2.50	0.45
2:E:384:GLU:HA	2:E:387:GLU:HG2	1.98	0.45
3:F:361:HIS:HD2	3:F:362:LYS:HG3	1.82	0.45
3:F:15:LEU:HA	3:F:106:ARG:NH2	2.31	0.45
1:D:79:ARG:HD2	3:F:311:ARG:HD2	1.98	0.45
1:D:137:SER:O	1:D:140:GLU:HB3	2.16	0.45
3:C:80:CYS:HB3	3:C:88:LEU:HD21	1.99	0.45
2:B:22:PHE:N	2:B:355:ASN:OD1	2.47	0.45
3:C:4:GLN:HE21	3:C:47:ASP:CG	2.21	0.45
3:F:16:LEU:O	3:F:18:LYS:HE2	2.18	0.45
3:C:310:GLU:CG	3:C:312:MET:HB2	2.45	0.44
3:C:126:THR:HB	7:C:502:GOL:O2	2.18	0.44
1:A:10:PHE:C	3:C:311:ARG:HH21	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:402:ILE:O	3:F:406:VAL:HG22	2.16	0.44
1:A:207:LEU:HD22	1:A:246:TYR:CD2	2.51	0.44
2:B:327:ASP:OD1	2:B:327:ASP:N	2.43	0.44
3:C:272:CYS:SG	3:C:294:ALA:HB1	2.57	0.44
1:A:224:LYS:HD2	1:A:251:ASP:CG	2.37	0.44
3:C:306:ALA:O	3:C:309:LYS:HG2	2.18	0.44
1:A:114:LEU:HD23	1:A:115:PRO:HD2	2.00	0.44
1:A:22:SER:HB2	1:A:112:PHE:HB3	2.00	0.44
1:D:118:GLU:HA	1:D:121:LYS:HB3	2.00	0.44
3:C:302:GLY:HA2	3:C:319:PHE:CE1	2.53	0.44
2:E:253:LEU:HD23	2:E:253:LEU:HA	1.62	0.44
1:A:215:LEU:HD22	1:A:225:VAL:HG13	1.98	0.44
3:C:185:THR:O	3:C:186:TYR:HB3	2.18	0.44
2:E:169:LEU:HA	2:E:169:LEU:HD23	1.68	0.44
3:C:36:LEU:O	3:C:37:ILE:HD13	2.18	0.44
2:B:292:ASP:HB2	2:B:293:GLU:HG3	2.00	0.44
3:C:114:CYS:SG	3:C:161:VAL:HG22	2.57	0.44
3:C:2:ILE:HG12	3:C:49:VAL:HG22	1.99	0.44
1:D:277:GLN:O	1:D:279:LYS:HG2	2.18	0.44
3:C:77:LEU:HA	3:C:77:LEU:HD23	1.70	0.44
2:E:139:TYR:CE2	3:F:65:ILE:HG22	2.52	0.44
1:A:146:LEU:CD2	1:A:150:LYS:HD2	2.48	0.44
2:E:238:LYS:NZ	2:E:359:LEU:O	2.30	0.44
3:C:304:TYR:O	3:C:308:LEU:HD12	2.18	0.43
3:F:242:ILE:CD1	3:F:422:ILE:HG23	2.48	0.43
1:D:126:ARG:CD	1:D:132:LYS:HZ3	2.31	0.43
1:D:148:TYR:O	1:D:151:GLU:HB3	2.18	0.43
3:F:280:ARG:HD3	8:F:605:HOH:O	2.18	0.43
2:E:118:GLN:HG3	2:E:237:LEU:HG	2.00	0.43
3:C:101:TRP:HA	3:C:101:TRP:CE3	2.53	0.43
3:F:144:ILE:HG22	3:F:146:PRO:HD3	2.00	0.43
2:E:117:ILE:HD13	2:E:258:ILE:HD11	1.99	0.43
1:D:2:SER:OG	3:F:327:GLU:OE1	2.36	0.43
1:A:209:THR:N	1:A:210:PRO:HD2	2.33	0.43
3:C:113:PRO:HA	3:C:159:LYS:O	2.18	0.43
3:F:137:ARG:HB2	3:F:138:TYR:CD1	2.53	0.43
3:C:142:ILE:HA	3:C:142:ILE:HD13	1.81	0.43
2:E:91:LEU:HB3	2:E:96:CYS:SG	2.59	0.43
3:F:218:ILE:HG21	3:F:224:PHE:HB2	2.01	0.43
1:D:135:PRO:HD2	1:D:138:ALA:HB3	1.99	0.43
1:D:178:LYS:HB2	1:D:223:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:243:ASP:OD1	2:E:243:ASP:N	2.50	0.43
2:B:168:TYR:O	2:B:172:VAL:HG23	2.18	0.43
3:C:170:PHE:O	3:C:174:THR:HG23	2.19	0.43
2:B:25:THR:OG1	2:B:387:GLU:OE2	2.19	0.43
2:E:253:LEU:HD11	2:E:265:HIS:HD2	1.83	0.43
1:D:240:GLU:OE1	1:D:250:TYR:OH	2.35	0.43
3:F:188:ASP:OD1	3:F:190:HIS:N	2.38	0.43
3:F:402:ILE:HG13	3:F:431:VAL:HG11	2.01	0.43
3:C:1:MET:HA	3:C:1:MET:HE3	2.01	0.43
1:D:123:CYS:HB3	1:D:134:ILE:CG2	2.48	0.43
1:A:137:SER:OG	1:A:138:ALA:N	2.52	0.43
1:D:90:SER:OG	1:D:91:LEU:N	2.48	0.43
2:E:121:LEU:HD23	2:E:127:LEU:HB2	2.00	0.43
2:E:139:TYR:HB2	3:F:67:PHE:HD2	1.83	0.43
1:A:86:ALA:HA	1:A:97:MET:CE	2.48	0.43
3:F:3:LEU:CD1	3:F:118:VAL:HG22	2.48	0.43
2:B:91:LEU:CD2	2:B:96:CYS:SG	3.07	0.43
3:F:304:TYR:O	3:F:308:LEU:HD12	2.19	0.43
3:F:104:ARG:HD2	3:F:104:ARG:HA	1.54	0.43
3:C:50:PHE:CE2	3:C:52:ASP:HB2	2.54	0.42
3:F:142:ILE:HG23	3:F:154:LEU:HD11	2.01	0.42
3:C:415:TYR:CE2	3:C:431:VAL:HG22	2.53	0.42
2:B:268:PHE:O	2:B:270:ASP:N	2.48	0.42
3:C:399:GLN:HG2	3:C:415:TYR:CZ	2.54	0.42
2:B:159:LEU:HD22	2:B:198:ILE:HG23	1.99	0.42
3:F:261:LEU:HD22	3:F:333:ASN:HB3	2.01	0.42
2:B:127:LEU:HD12	2:B:127:LEU:HA	1.57	0.42
1:A:184:LEU:HD23	1:A:231:ARG:NH2	2.35	0.42
2:E:137:SER:HB3	2:E:220:LEU:HD21	2.01	0.42
1:A:236:ARG:O	1:A:240:GLU:HG2	2.19	0.42
3:C:344:THR:O	3:C:348:ALA:N	2.52	0.42
1:A:24:LYS:HE3	4:A:401:PO4:O1	2.20	0.42
2:E:266:TYR:CE2	2:E:277:LYS:HD3	2.55	0.42
2:E:256:GLN:HB3	2:E:263:PHE:CZ	2.54	0.42
2:B:178:LEU:HB2	2:B:183:LEU:HD23	2.02	0.42
3:F:142:ILE:HD11	3:F:171:ILE:HD11	2.00	0.42
3:C:83:PHE:HB3	3:C:84:PHE:CE1	2.55	0.42
2:B:243:ASP:HB2	2:B:245:ARG:H	1.83	0.42
1:A:120:VAL:HG12	1:A:139:ILE:HD12	2.02	0.42
1:D:8:HIS:CD2	1:D:8:HIS:N	2.88	0.42
3:C:185:THR:HG22	3:C:186:TYR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LYS:HB3	2:B:268:PHE:HB2	2.01	0.42
3:F:55:TYR:CZ	3:F:60:GLU:HG3	2.55	0.42
3:F:283:ARG:NH1	3:F:283:ARG:HG3	2.34	0.42
3:C:62:SER:HB3	3:C:184:TYR:CD2	2.54	0.42
1:D:8:HIS:C	1:D:9:HIS:CD2	2.93	0.42
2:B:90:HIS:O	2:B:91:LEU:HB3	2.20	0.42
1:D:243:LEU:HD13	1:D:250:TYR:CE2	2.55	0.42
3:F:334:ILE:HB	3:F:363:MET:HG3	2.02	0.42
1:D:235:TYR:O	1:D:238:PRO:HD2	2.19	0.41
3:F:313:GLU:HB3	3:F:315:ASP:OD2	2.20	0.41
2:B:74:ARG:O	2:B:77:ASP:HB2	2.19	0.41
3:F:275:LEU:HB3	3:F:278:TYR:HB3	2.01	0.41
1:D:195:ASP:HB3	1:D:198:ASN:HB3	2.02	0.41
2:E:90:HIS:HE1	2:E:127:LEU:HD12	1.85	0.41
2:B:246:GLU:OE1	2:B:362:PRO:HA	2.21	0.41
2:E:253:LEU:HD11	2:E:265:HIS:CD2	2.55	0.41
2:B:246:GLU:OE2	2:B:363:TYR:N	2.39	0.41
3:C:134:MET:HE1	3:C:377:PHE:HB2	2.02	0.41
2:B:345:LEU:HD12	2:B:345:LEU:O	2.20	0.41
3:F:317:LEU:HD12	3:F:317:LEU:HA	1.76	0.41
1:D:16:LEU:HB3	1:D:24:LYS:HG2	2.03	0.41
3:F:121:LEU:HD23	3:F:152:LEU:HD11	2.01	0.41
2:B:23:SER:HB3	2:B:66:TYR:CE1	2.55	0.41
2:E:54:LYS:O	2:E:267:GLN:HA	2.21	0.41
3:F:195:TYR:O	3:F:198:ILE:HG13	2.21	0.41
3:C:5:ILE:O	3:C:45:GLN:HA	2.21	0.41
2:B:163:GLN:HA	2:B:168:TYR:CE1	2.56	0.41
3:F:174:THR:O	3:F:178:THR:HG23	2.20	0.41
3:C:101:TRP:O	3:C:102:LEU:HD23	2.21	0.41
3:C:283:ARG:HB2	3:C:286:TYR:CD2	2.56	0.41
1:A:303:PRO:HB3	1:D:210:PRO:HG3	2.03	0.41
2:B:391:ASP:HB3	2:B:394:LEU:HG	2.03	0.41
1:D:179:ALA:O	1:D:282:VAL:HA	2.21	0.41
1:A:31:PHE:CZ	1:A:35:GLU:HG3	2.55	0.41
2:E:136:PHE:CE1	2:E:220:LEU:HD11	2.53	0.41
3:F:154:LEU:HD12	3:F:155:ARG:H	1.86	0.41
1:A:305:PHE:CE1	1:D:307:VAL:HG13	2.56	0.41
1:D:157:PRO:O	1:D:158:ILE:HD13	2.21	0.41
1:A:219:LYS:HE3	1:A:219:LYS:HB2	1.93	0.41
1:A:12:LYS:HE2	1:A:12:LYS:HB3	1.87	0.41
1:D:178:LYS:HB2	1:D:223:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:323:VAL:HG23	2:E:324:TYR:HD2	1.85	0.41
1:A:270:GLU:O	1:A:274:GLU:HG3	2.21	0.41
1:A:127:CYS:HA	1:A:129:GLN:NE2	2.35	0.41
1:A:146:LEU:O	1:A:150:LYS:HB2	2.21	0.41
3:C:1:MET:HE3	3:C:2:ILE:H	1.86	0.41
1:A:37:ASN:O	1:A:81:ASN:HB2	2.20	0.41
1:D:59:PHE:HE1	1:D:63:ARG:CZ	2.33	0.41
1:A:13:LEU:HD12	1:A:82:VAL:O	2.21	0.41
3:C:133:PHE:HB2	3:C:144:ILE:HG12	2.03	0.41
2:B:343:GLY:HA2	2:B:346:ARG:HB3	2.03	0.41
2:B:150:LEU:HA	2:B:150:LEU:HD23	1.81	0.41
3:F:181:TYR:HB2	3:F:185:THR:HG21	2.03	0.41
2:B:131:LEU:HA	2:B:131:LEU:HD12	1.89	0.41
3:C:86:GLU:CD	3:C:86:GLU:H	2.24	0.41
2:B:81:VAL:HG12	2:B:87:LYS:HA	2.03	0.40
3:F:261:LEU:HA	3:F:261:LEU:HD23	1.80	0.40
3:C:228:LYS:HE3	3:C:232:GLU:OE2	2.21	0.40
2:E:72:HIS:ND1	2:E:77:ASP:HB3	2.36	0.40
2:B:191:ILE:HD13	2:B:191:ILE:HA	1.74	0.40
3:C:205:VAL:HA	3:C:206:PRO:HD2	1.92	0.40
1:D:265:ASN:HD21	1:D:291:GLN:HB3	1.86	0.40
1:A:10:PHE:O	3:C:311:ARG:NH2	2.55	0.40
3:F:58:LEU:HD13	3:F:68:GLN:HG3	2.03	0.40
2:E:310:PRO:HB3	2:E:352:TRP:CE2	2.57	0.40
2:B:75:LEU:HD12	2:B:104:HIS:CD2	2.56	0.40
2:E:278:TYR:HB3	2:E:279:PRO:HD3	2.03	0.40
3:C:129:SER:HB2	3:C:130:LYS:HD3	2.03	0.40
1:D:119:LEU:HD23	1:D:119:LEU:HA	1.93	0.40
3:C:336:LEU:HD12	3:C:339:VAL:CG2	2.52	0.40
2:E:253:LEU:HD12	2:E:301:ARG:NE	2.36	0.40
1:A:30:TYR:CE1	2:B:374:LYS:HB3	2.56	0.40
2:B:24:PRO:HA	2:B:380:ARG:HH21	1.85	0.40
3:F:135:MET:HG2	8:F:616:HOH:O	2.20	0.40
1:A:181:ILE:HA	1:A:226:ILE:O	2.22	0.40
1:D:262:ARG:HH22	1:D:270:GLU:CD	2.25	0.40
2:B:121:LEU:HD13	2:B:231:PHE:CE2	2.57	0.40
3:C:406:VAL:HG13	3:C:409:THR:OG1	2.21	0.40
1:D:263:LYS:O	1:D:266:ILE:HG22	2.22	0.40
3:F:48:VAL:HG11	3:F:79:ILE:HG12	2.02	0.40
3:C:402:ILE:HG13	3:C:431:VAL:HG21	2.04	0.40
3:F:228:LYS:HE3	3:F:232:GLU:OE2	2.22	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	309/312 (99%)	267 (86%)	35 (11%)	7 (2%)	8	39
1	D	309/312 (99%)	266 (86%)	38 (12%)	5 (2%)	12	48
2	B	392/394 (100%)	359 (92%)	31 (8%)	2 (0%)	34	71
2	E	391/394 (99%)	359 (92%)	31 (8%)	1 (0%)	46	81
3	C	420/436 (96%)	384 (91%)	32 (8%)	4 (1%)	19	58
3	F	418/436 (96%)	386 (92%)	28 (7%)	4 (1%)	19	58
All	All	2239/2284 (98%)	2021 (90%)	195 (9%)	23 (1%)	19	58

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	127	CYS
1	A	132	LYS
3	C	185	THR
3	C	188	ASP
1	D	90	SER
2	E	90	HIS
3	C	103	GLU
1	D	55	LEU
3	F	185	THR
3	F	313	GLU
1	A	125	LYS
2	B	90	HIS
1	D	163	LYS
1	A	126	ARG
1	A	153	PHE
1	A	91	LEU

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Mol	Chain	Res	Type
3	C	186	TYR
1	D	125	LYS
2	B	180	ALA
3	F	188	ASP
3	F	315	ASP
1	D	237	GLU

### 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	282/283 (100%)	277 (98%)	5 (2%)	66	85
1	D	282/283 (100%)	276 (98%)	6 (2%)	61	84
2	B	358/358 (100%)	347 (97%)	11 (3%)	47	79
2	E	357/358 (100%)	353 (99%)	4 (1%)	80	90
3	C	387/399 (97%)	380 (98%)	7 (2%)	66	85
3	F	385/399 (96%)	379 (98%)	6 (2%)	70	87
All	All	2051/2080 (99%)	2012 (98%)	39 (2%)	65	85

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	87	THR
1	A	122	ARG
1	A	129	GLN
1	A	163	LYS
2	B	22	PHE
2	B	36	ASN
2	B	83	ARG
2	B	84	ASN
2	B	140	TYR
2	B	154	SER
2	B	210	GLN

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Mol	Chain	Res	Type
2	B	243	ASP
2	B	262	ASP
2	B	339	ARG
2	B	364	SER
3	C	22	THR
3	C	65	ILE
3	C	150	ASN
3	C	160	SER
3	C	309	LYS
3	C	313	GLU
3	C	315	ASP
1	D	69	GLU
1	D	114	LEU
1	D	132	LYS
1	D	164	GLU
1	D	282	VAL
1	D	295	MET
2	E	154	SER
2	E	230	PHE
2	E	243	ASP
2	E	267	GLN
3	F	81	ASN
3	F	104	ARG
3	F	160	SER
3	F	247	THR
3	F	300	SER
3	F	337	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	221	GLN
2	B	265	HIS
3	C	4	GLN
3	C	89	GLN
3	C	97	GLN
3	C	150	ASN
3	C	390	HIS
1	D	5	ASN
1	D	9	HIS
1	D	172	GLN

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Mol	Chain	Res	Type
1	D	192	ASN
1	D	208	ASN
2	E	134	ASN
3	F	193	GLN

### 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 carbohydrates in this entry.

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

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	PO4	A	401	-	4,4,4	0.53	0	6,6,6	0.28	0
6	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.24	0
6	SO4	A	404	-	4,4,4	0.16	0	6,6,6	0.08	0
6	SO4	B	403	-	4,4,4	0.30	0	6,6,6	0.54	0
7	GOL	B	404	-	5,5,5	0.53	0	5,5,5	1.07	0
6	SO4	C	501	-	4,4,4	0.18	0	6,6,6	0.19	0
7	GOL	C	502	-	5,5,5	0.29	0	5,5,5	0.36	0
7	GOL	C	503	-	5,5,5	0.38	0	5,5,5	0.35	0
7	GOL	C	504	-	5,5,5	0.52	0	5,5,5	0.40	0
4	PO4	D	401	-	4,4,4	0.53	0	6,6,6	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	E	401	-	4,4,4	0.15	0	6,6,6	0.40	0
6	SO4	E	402	-	4,4,4	0.16	0	6,6,6	0.25	0
6	SO4	F	501	-	4,4,4	0.17	0	6,6,6	0.39	0
6	SO4	F	502	-	4,4,4	0.20	0	6,6,6	0.34	0
7	GOL	F	503	-	5,5,5	0.52	0	5,5,5	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	A	401	-	-	0/0/0/0	0/0/0/0
6	SO4	A	403	-	-	0/0/0/0	0/0/0/0
6	SO4	A	404	-	-	0/0/0/0	0/0/0/0
6	SO4	B	403	-	-	0/0/0/0	0/0/0/0
7	GOL	B	404	-	-	0/4/4/4	0/0/0/0
6	SO4	C	501	-	-	0/0/0/0	0/0/0/0
7	GOL	C	502	-	-	0/4/4/4	0/0/0/0
7	GOL	C	503	-	-	0/4/4/4	0/0/0/0
7	GOL	C	504	-	-	0/4/4/4	0/0/0/0
4	PO4	D	401	-	-	0/0/0/0	0/0/0/0
6	SO4	E	401	-	-	0/0/0/0	0/0/0/0
6	SO4	E	402	-	-	0/0/0/0	0/0/0/0
6	SO4	F	501	-	-	0/0/0/0	0/0/0/0
6	SO4	F	502	-	-	0/0/0/0	0/0/0/0
7	GOL	F	503	-	-	0/4/4/4	0/0/0/0

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.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	PO4	2	0
6	B	403	SO4	1	0
7	B	404	GOL	1	0
7	C	502	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	503	GOL	1	0
7	F	503	GOL	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	311/312 (99%)	-0.02	4 (1%) 79 74	38, 77, 131, 191	0
1	D	311/312 (99%)	-0.01	1 (0%) 94 94	46, 75, 126, 167	0
2	B	394/394 (100%)	-0.32	1 (0%) 94 94	35, 53, 91, 126	0
2	E	393/394 (99%)	-0.09	1 (0%) 94 94	44, 77, 118, 137	0
3	C	424/436 (97%)	-0.26	1 (0%) 95 95	35, 60, 103, 148	0
3	F	422/436 (96%)	-0.27	1 (0%) 95 95	40, 60, 98, 158	0
All	All	2255/2284 (98%)	-0.18	9 (0%) 93 92	35, 66, 115, 191	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	ILE	3.1
1	A	134	ILE	3.0
2	B	1	MET	3.0
1	D	139	ILE	2.7
1	A	2	SER	2.6
3	F	185	THR	2.5
2	E	274	PHE	2.3
1	A	252	LEU	2.3
3	C	185	THR	2.1

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	F	502	5/5	0.83	0.42	22.52	135,137,143,144	0
5	MG	A	402	1/1	0.98	0.39	8.93	58,58,58,58	0
7	GOL	C	504	6/6	0.86	0.36	6.43	53,67,72,75	0
6	SO4	C	501	5/5	0.91	0.30	6.08	125,126,127,129	0
7	GOL	B	404	6/6	0.82	0.37	5.11	55,68,75,81	0
6	SO4	E	401	5/5	0.85	0.39	4.94	123,124,126,127	0
6	SO4	A	403	5/5	0.86	0.43	4.03	143,148,149,150	0
5	MG	D	402	1/1	0.98	0.34	3.56	43,43,43,43	0
7	GOL	C	503	6/6	0.52	0.37	2.09	83,87,95,96	0
7	GOL	C	502	6/6	0.94	0.29	1.40	73,78,80,83	0
6	SO4	F	501	5/5	0.80	0.25	0.17	135,139,140,141	0
7	GOL	F	503	6/6	0.93	0.16	-0.15	56,67,74,77	0
5	MG	B	402	1/1	0.94	0.23	-0.18	41,41,41,41	0
4	PO4	A	401	5/5	0.99	0.15	-0.54	51,58,62,71	0
4	PO4	D	401	5/5	0.96	0.13	-1.18	56,60,68,71	0
6	SO4	B	403	5/5	0.98	0.11	-1.64	70,70,73,74	0
6	SO4	A	404	5/5	0.91	0.30	-	168,169,171,171	0
5	MG	B	401	1/1	0.86	0.13	-	42,42,42,42	0
6	SO4	E	402	5/5	0.97	0.07	-	90,93,95,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.