



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:42 AM GMT

PDB ID : 2I9B  
Title : Crystal structure of ATF-urokinase receptor complex  
Authors : Lubkowski, J.; Barinka, C.  
Deposited on : 2006-09-05  
Resolution : 2.80 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

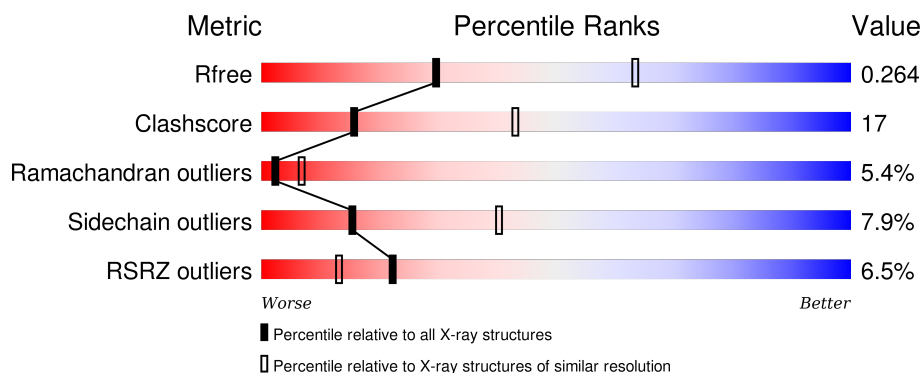
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	145	
1	B	145	
1	C	145	
1	D	145	
2	E	279	

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Mol	Chain	Length	Quality of chain
2	F	279	
2	G	279	
2	H	279	

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
5	SO4	E	318	-	-	X	-
5	SO4	F	328	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11892 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 Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			966	596	183	173	14			
1	B	122	Total	C	N	O	S	0	0	0
			966	596	183	173	14			
1	C	122	Total	C	N	O	S	0	0	0
			966	596	183	173	14			
1	D	122	Total	C	N	O	S	0	0	0
			966	596	183	173	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	CLONING ARTIFACT	UNP P00749
A	0	SER	-	CLONING ARTIFACT	UNP P00749
B	-1	ARG	-	CLONING ARTIFACT	UNP P00749
B	0	SER	-	CLONING ARTIFACT	UNP P00749
C	-1	ARG	-	CLONING ARTIFACT	UNP P00749
C	0	SER	-	CLONING ARTIFACT	UNP P00749
D	-1	ARG	-	CLONING ARTIFACT	UNP P00749
D	0	SER	-	CLONING ARTIFACT	UNP P00749

- Molecule 2 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	265	Total	C	N	O	S	0	0	0
			2034	1222	374	406	32			
2	F	265	Total	C	N	O	S	0	0	0
			2034	1222	374	406	32			
2	G	248	Total	C	N	O	S	0	0	0
			1882	1127	344	379	32			
2	H	248	Total	C	N	O	S	0	0	0
			1882	1127	344	379	32			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ARG	-	CLONING ARTIFACT	UNP Q03405
E	0	SER	-	CLONING ARTIFACT	UNP Q03405
E	162	GLN	ASN	ENGINEERED	UNP Q03405
E	172	GLN	ASN	ENGINEERED	UNP Q03405
E	200	GLN	ASN	ENGINEERED	UNP Q03405
E	233	GLN	ASN	ENGINEERED	UNP Q03405
F	-1	ARG	-	CLONING ARTIFACT	UNP Q03405
F	0	SER	-	CLONING ARTIFACT	UNP Q03405
F	162	GLN	ASN	ENGINEERED	UNP Q03405
F	172	GLN	ASN	ENGINEERED	UNP Q03405
F	200	GLN	ASN	ENGINEERED	UNP Q03405
F	233	GLN	ASN	ENGINEERED	UNP Q03405
G	-1	ARG	-	CLONING ARTIFACT	UNP Q03405
G	0	SER	-	CLONING ARTIFACT	UNP Q03405
G	162	GLN	ASN	ENGINEERED	UNP Q03405
G	172	GLN	ASN	ENGINEERED	UNP Q03405
G	200	GLN	ASN	ENGINEERED	UNP Q03405
G	233	GLN	ASN	ENGINEERED	UNP Q03405
H	-1	ARG	-	CLONING ARTIFACT	UNP Q03405
H	0	SER	-	CLONING ARTIFACT	UNP Q03405
H	162	GLN	ASN	ENGINEERED	UNP Q03405
H	172	GLN	ASN	ENGINEERED	UNP Q03405
H	200	GLN	ASN	ENGINEERED	UNP Q03405
H	233	GLN	ASN	ENGINEERED	UNP Q03405

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

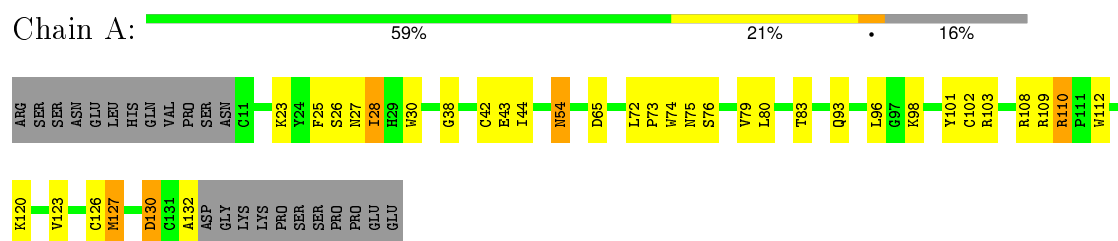
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	13	Total	O	0	0
			13	13		
6	C	3	Total	O	0	0
			3	3		
6	D	2	Total	O	0	0
			2	2		
6	E	11	Total	O	0	0
			11	11		
6	F	7	Total	O	0	0
			7	7		
6	G	2	Total	O	0	0
			2	2		

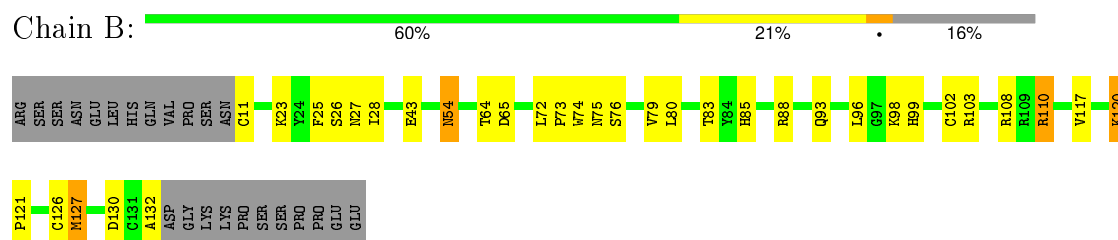
### 3 Residue-property plots [i](#)

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.

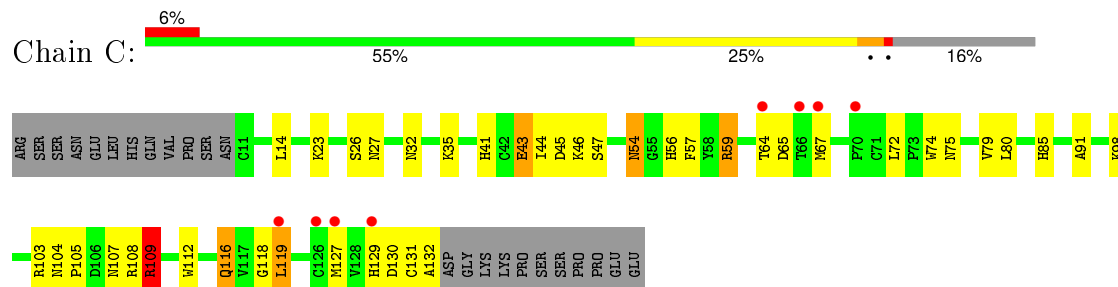
- Molecule 1: Urokinase-type plasminogen activator



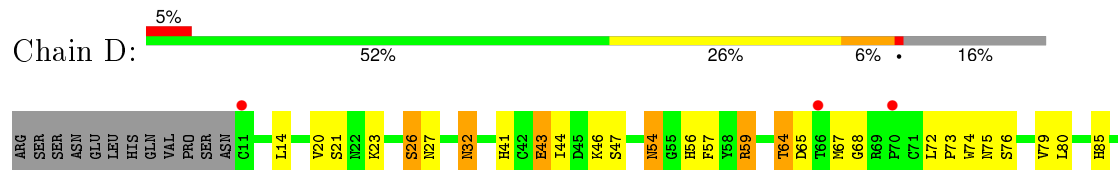
- Molecule 1: Urokinase-type plasminogen activator



- Molecule 1: Urokinase-type plasminogen activator

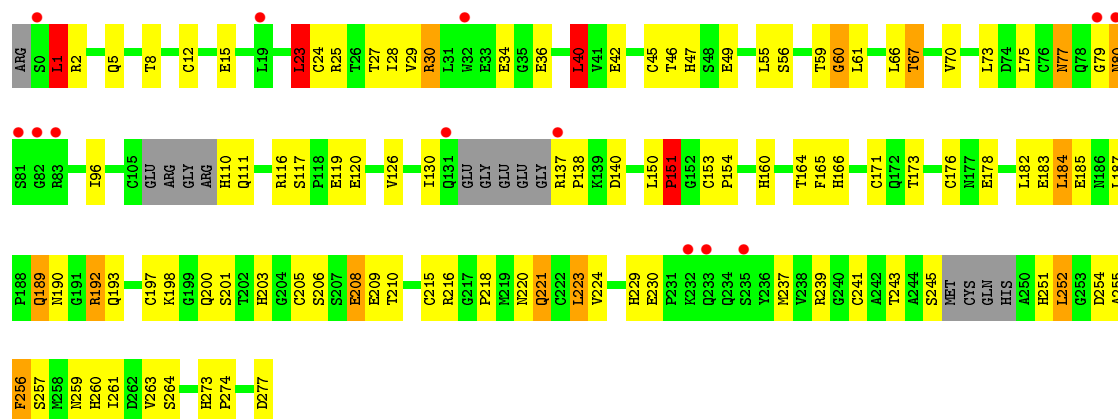


- Molecule 1: Urokinase-type plasminogen activator

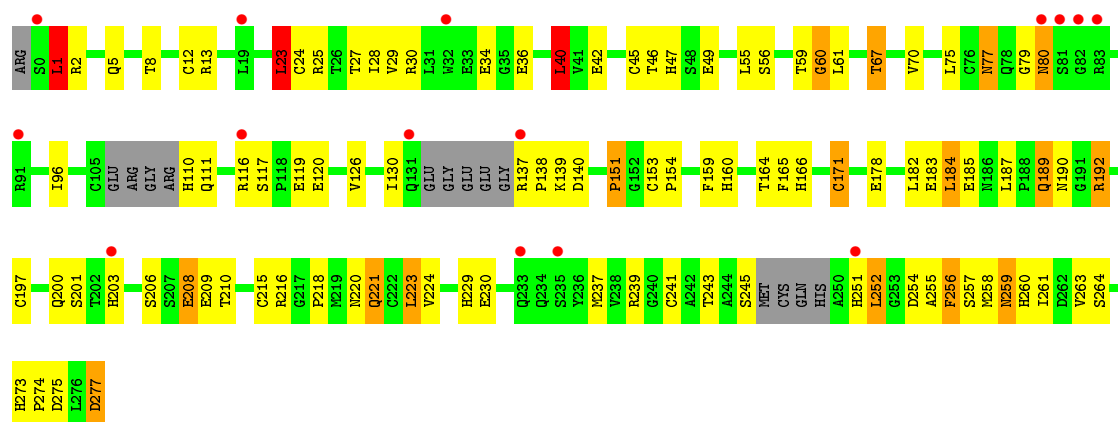




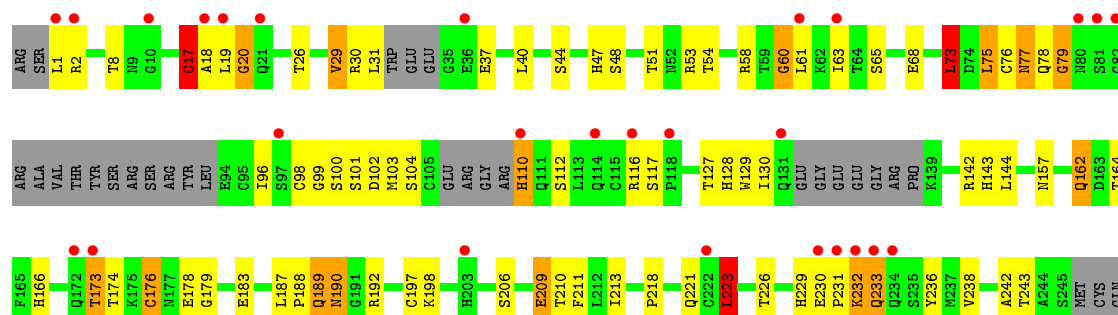
• Molecule 2: Urokinase plasminogen activator surface receptor



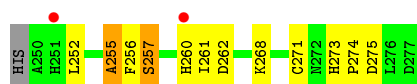
• Molecule 2: Urokinase plasminogen activator surface receptor



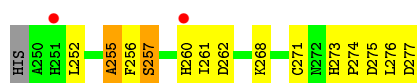
• Molecule 2: Urokinase plasminogen activator surface receptor







● Molecule 2: Urokinase plasminogen activator surface receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.91Å 281.92Å 62.81Å 90.00° 105.41° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (15.00-2.80) 91.2 (14.98-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.222 , 0.265 0.221 , 0.264	Depositor DCC
$R_{free}$ test set	1911 reflections (4.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.5	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 86.4	EDS
Estimated twinning fraction	0.468 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 46704 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	0.60	0/993	0.85	0/1342
1	B	0.62	0/993	0.86	0/1342
1	C	0.48	0/993	0.77	1/1342 (0.1%)
1	D	0.59	0/993	0.81	1/1342 (0.1%)
2	E	0.66	1/2065 (0.0%)	1.00	6/2780 (0.2%)
2	F	0.66	2/2065 (0.1%)	0.98	5/2780 (0.2%)
2	G	0.56	1/1906 (0.1%)	0.89	2/2561 (0.1%)
2	H	0.56	1/1906 (0.1%)	0.88	2/2561 (0.1%)
All	All	0.60	5/11914 (0.0%)	0.90	17/16050 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	176	CYS	CB-SG	-6.75	1.70	1.82
2	H	176	CYS	CB-SG	-6.33	1.71	1.82
2	E	49	GLU	CG-CD	5.25	1.59	1.51
2	F	49	GLU	CG-CD	5.19	1.59	1.51
2	F	171	CYS	CB-SG	-5.19	1.73	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	223	LEU	CA-CB-CG	6.49	130.22	115.30
2	G	223	LEU	CA-CB-CG	5.86	128.78	115.30
2	F	61	LEU	CA-CB-CG	5.77	128.56	115.30
2	H	223	LEU	CA-CB-CG	5.73	128.48	115.30
2	F	1	LEU	CA-CB-CG	5.72	128.47	115.30
2	F	223	LEU	CA-CB-CG	5.69	128.39	115.30
2	E	40	LEU	CA-CB-CG	5.60	128.17	115.30
1	D	109	ARG	NE-CZ-NH2	5.57	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	LEU	CA-CB-CG	5.54	128.05	115.30
2	E	23	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	109	ARG	NE-CZ-NH2	5.45	123.03	120.30
2	E	61	LEU	CA-CB-CG	5.40	127.72	115.30
2	F	23	LEU	CA-CB-CG	5.38	127.68	115.30
2	E	73	LEU	CA-CB-CG	5.35	127.60	115.30
2	G	144	LEU	CA-CB-CG	5.06	126.94	115.30
2	H	144	LEU	CA-CB-CG	5.05	126.91	115.30
2	F	40	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	966	0	900	31	0
1	B	966	0	900	30	0
1	C	966	0	900	27	0
1	D	966	0	900	34	0
2	E	2034	0	1908	69	0
2	F	2034	0	1908	69	0
2	G	1882	0	1760	73	0
2	H	1882	0	1761	75	0
3	E	39	0	34	1	0
3	F	39	0	34	1	0
4	G	28	0	25	0	0
4	H	28	0	25	1	0
5	E	5	0	0	4	0
5	F	5	0	0	3	0
6	A	14	0	0	0	0
6	B	13	0	0	1	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
6	E	11	0	0	0	0
6	F	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	2	0	0	0	0
All	All	11892	0	11055	391	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:HIS:NE2	2:H:260:HIS:CE1	2.24	1.06
2:G:47:HIS:NE2	2:G:260:HIS:CE1	2.25	1.03
2:E:137:ARG:HG2	2:E:138:PRO:HD3	1.37	1.01
2:F:137:ARG:HG2	2:F:138:PRO:HD3	1.44	0.99
2:G:47:HIS:NE2	2:G:260:HIS:HE1	1.71	0.88
2:H:47:HIS:CD2	2:H:260:HIS:CE1	2.62	0.86
2:E:263:VAL:HG12	2:E:264:SER:H	1.40	0.86
2:G:47:HIS:CD2	2:G:260:HIS:CE1	2.63	0.85
2:F:130:ILE:HG21	2:F:166:HIS:HE2	1.41	0.84
2:H:47:HIS:NE2	2:H:260:HIS:HE1	1.73	0.84
2:G:103:MET:HG3	2:H:103:MET:HG3	1.61	0.83
2:F:263:VAL:HG12	2:F:264:SER:H	1.42	0.82
2:F:263:VAL:HG12	2:F:264:SER:N	1.93	0.82
2:E:130:ILE:HG21	2:E:166:HIS:HE2	1.46	0.81
2:E:263:VAL:HG12	2:E:264:SER:N	1.98	0.79
1:B:108:ARG:NH2	1:D:105:PRO:O	2.12	0.78
2:H:173:THR:O	2:H:176:CYS:HB2	1.82	0.78
2:H:47:HIS:HE1	2:H:233:GLN:NE2	1.82	0.78
1:D:54:ASN:HD22	1:D:54:ASN:H	1.30	0.78
2:G:162:GLN:HG2	2:G:211:PHE:HE1	1.49	0.77
1:C:54:ASN:H	1:C:54:ASN:HD22	1.33	0.77
2:G:47:HIS:HE1	2:G:233:GLN:NE2	1.81	0.77
2:G:162:GLN:HG2	2:G:211:PHE:CE1	2.20	0.77
2:F:229:HIS:CD2	2:F:230:GLU:HG2	2.18	0.77
2:E:229:HIS:CD2	2:E:230:GLU:HG2	2.20	0.76
2:F:197:CYS:HB3	2:F:210:THR:HG22	1.68	0.76
2:G:96:ILE:HD13	2:G:110:HIS:HD2	1.51	0.76
2:E:197:CYS:HB3	2:E:210:THR:HG22	1.67	0.75
2:F:59:THR:O	2:F:59:THR:HG22	1.84	0.75
2:H:96:ILE:HD13	2:H:110:HIS:HD2	1.52	0.75
1:D:104:ASN:HD21	1:D:108:ARG:H	1.34	0.74
2:E:47:HIS:ND1	5:E:318:SO4:O4	2.15	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:CYS:O	1:A:103:ARG:NH1	2.22	0.73
1:B:102:CYS:O	1:B:103:ARG:NH1	2.21	0.72
2:E:130:ILE:O	2:E:130:ILE:HG23	1.89	0.72
2:F:60:GLY:H	2:F:111:GLN:HE22	1.36	0.72
3:E:311:NAG:H61	3:E:312:NAG:HN2	1.54	0.72
1:B:25:PHE:HB2	1:B:28:ILE:HD11	1.71	0.71
2:E:59:THR:O	2:E:59:THR:HG22	1.91	0.70
2:G:173:THR:O	2:G:176:CYS:HB2	1.92	0.70
1:A:108:ARG:NH2	1:C:105:PRO:O	2.21	0.70
2:F:28:ILE:HG21	2:F:30:ARG:HH11	1.56	0.70
2:E:200:GLN:HB2	2:E:203:HIS:HB2	1.72	0.69
2:G:99:GLY:H	2:G:104:SER:HB2	1.57	0.69
2:F:117:SER:HB2	2:F:120:GLU:HG3	1.73	0.69
1:C:104:ASN:HD21	1:C:108:ARG:H	1.38	0.69
2:F:200:GLN:HB2	2:F:203:HIS:HB2	1.75	0.69
2:E:60:GLY:H	2:E:111:GLN:HE22	1.41	0.69
2:F:206:SER:OG	2:F:209:GLU:HG3	1.94	0.68
2:G:47:HIS:CE1	2:G:233:GLN:NE2	2.61	0.68
2:G:29:VAL:HG13	2:G:40:LEU:HB2	1.75	0.68
2:H:47:HIS:CE1	2:H:233:GLN:NE2	2.61	0.68
2:E:130:ILE:HG21	2:E:166:HIS:NE2	2.08	0.68
2:E:137:ARG:HG2	2:E:138:PRO:CD	2.21	0.68
2:F:130:ILE:HG21	2:F:166:HIS:NE2	2.07	0.68
2:F:263:VAL:CG1	2:F:264:SER:H	2.07	0.68
2:F:237:MET:SD	2:F:239:ARG:NH1	2.67	0.67
2:H:29:VAL:HG13	2:H:40:LEU:HB2	1.77	0.67
2:F:189:GLN:HE21	2:F:189:GLN:HA	1.58	0.67
2:F:229:HIS:HD2	2:F:230:GLU:HG2	1.58	0.67
2:G:162:GLN:HE21	2:G:213:ILE:HD11	1.58	0.67
2:E:229:HIS:HD2	2:E:230:GLU:HG2	1.59	0.66
2:F:130:ILE:HG23	2:F:130:ILE:O	1.94	0.66
1:A:25:PHE:HB2	1:A:28:ILE:HD11	1.78	0.66
1:C:109:ARG:HG3	1:C:109:ARG:HH21	1.58	0.66
1:A:54:ASN:HD22	1:A:54:ASN:H	1.40	0.66
2:G:130:ILE:HG21	2:G:166:HIS:HE1	1.60	0.66
2:E:206:SER:OG	2:E:209:GLU:HG3	1.96	0.66
2:E:208:GLU:OE1	2:E:208:GLU:N	2.27	0.66
2:E:189:GLN:HE21	2:E:189:GLN:HA	1.60	0.65
2:H:130:ILE:HG21	2:H:166:HIS:HE1	1.61	0.65
2:E:237:MET:SD	2:E:239:ARG:NH1	2.69	0.65
2:H:99:GLY:H	2:H:104:SER:HB2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:117:SER:HB2	2:E:120:GLU:HG3	1.78	0.65
2:F:47:HIS:ND1	5:F:328:SO4:O2	2.26	0.64
1:A:75:ASN:ND2	1:A:98:LYS:HG2	2.12	0.64
2:E:263:VAL:CG1	2:E:264:SER:H	2.09	0.64
2:H:268:LYS:O	2:H:271:CYS:SG	2.56	0.64
2:G:47:HIS:HE1	2:G:233:GLN:CD	2.01	0.64
1:D:64:THR:OG1	1:D:68:GLY:HA2	1.97	0.64
1:B:54:ASN:HD22	1:B:54:ASN:H	1.45	0.63
3:F:321:NAG:H61	3:F:322:NAG:HN2	1.63	0.63
2:F:218:PRO:O	2:F:243:THR:HG22	1.98	0.63
1:D:109:ARG:HG3	1:D:109:ARG:HH21	1.62	0.63
2:H:51:THR:H	2:H:53:ARG:HH11	1.45	0.63
1:A:27:ASN:HB2	2:E:42:GLU:OE2	1.98	0.63
1:C:109:ARG:CG	1:C:109:ARG:HH21	2.12	0.63
2:H:52:ASN:HD21	4:H:341:NAG:HN2	1.47	0.63
2:E:260:HIS:CE1	5:E:318:SO4:O3	2.52	0.63
2:G:31:LEU:O	2:G:37:GLU:HA	1.99	0.62
2:F:263:VAL:CG1	2:F:264:SER:N	2.62	0.62
2:G:268:LYS:O	2:G:271:CYS:SG	2.58	0.62
2:H:31:LEU:O	2:H:37:GLU:HA	2.00	0.62
1:B:75:ASN:ND2	1:B:98:LYS:HG2	2.14	0.62
1:D:72:LEU:HD21	1:D:116:GLN:HB2	1.82	0.61
1:A:76:SER:O	1:A:80:LEU:HG	2.01	0.61
2:H:47:HIS:HE1	2:H:233:GLN:CD	2.05	0.60
1:D:109:ARG:HH21	1:D:109:ARG:CG	2.13	0.60
1:D:14:LEU:HD12	1:D:43:GLU:HB3	1.83	0.60
2:E:218:PRO:O	2:E:243:THR:HG22	2.02	0.60
1:B:76:SER:O	1:B:80:LEU:HG	2.01	0.60
2:G:103:MET:CG	2:H:103:MET:HG3	2.30	0.59
2:F:190:ASN:ND2	2:F:192:ARG:HB3	2.16	0.59
1:B:117:VAL:O	1:B:120:LYS:HG2	2.01	0.59
2:H:223:LEU:HD23	2:H:242:ALA:CB	2.33	0.59
2:E:28:ILE:HG21	2:E:30:ARG:HH11	1.66	0.59
2:G:103:MET:HG3	2:H:103:MET:CG	2.31	0.58
2:F:137:ARG:HG2	2:F:138:PRO:CD	2.27	0.58
2:G:51:THR:H	2:G:53:ARG:HH11	1.51	0.58
1:C:14:LEU:HD12	1:C:43:GLU:HB3	1.83	0.58
2:E:130:ILE:CG2	2:E:130:ILE:O	2.51	0.58
2:F:29:VAL:HG12	2:F:40:LEU:HB2	1.86	0.58
2:G:130:ILE:HG21	2:G:166:HIS:CE1	2.38	0.58
2:F:25:ARG:HB3	2:F:70:VAL:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:TRP:HA	1:D:79:VAL:HG11	1.85	0.58
2:H:273:HIS:HD2	2:H:275:ASP:H	1.49	0.58
2:G:47:HIS:CE1	2:G:233:GLN:CD	2.77	0.58
2:F:208:GLU:N	2:F:208:GLU:OE1	2.29	0.57
2:F:273:HIS:ND1	2:F:274:PRO:HD2	2.19	0.57
2:E:190:ASN:ND2	2:E:192:ARG:HB3	2.19	0.57
1:C:72:LEU:HD21	1:C:116:GLN:HB2	1.87	0.56
1:C:74:TRP:HA	1:C:79:VAL:HG11	1.87	0.56
2:H:47:HIS:CE1	2:H:233:GLN:CD	2.79	0.56
2:G:96:ILE:HD13	2:G:110:HIS:CD2	2.37	0.56
2:H:130:ILE:HG21	2:H:166:HIS:CE1	2.38	0.56
1:D:41:HIS:HB2	1:D:43:GLU:HG3	1.87	0.56
2:F:184:LEU:HD22	2:F:216:ARG:HD2	1.88	0.56
2:G:273:HIS:HD2	2:G:275:ASP:H	1.53	0.56
2:E:29:VAL:HG12	2:E:40:LEU:HB2	1.88	0.56
1:D:54:ASN:HD21	1:D:56:HIS:HD2	1.52	0.55
2:F:59:THR:O	2:F:59:THR:CG2	2.54	0.55
2:E:206:SER:HG	2:E:209:GLU:HG3	1.71	0.55
1:D:118:GLY:O	1:D:119:LEU:HB2	2.07	0.55
2:F:260:HIS:ND1	5:F:328:SO4:O4	2.40	0.55
1:A:93:GLN:HG2	2:H:273:HIS:CD2	2.42	0.55
2:F:130:ILE:CG2	2:F:130:ILE:O	2.56	0.54
2:H:128:HIS:HB2	2:H:142:ARG:NH2	2.22	0.54
2:E:273:HIS:ND1	2:E:274:PRO:HD2	2.23	0.54
1:A:75:ASN:HD22	1:A:98:LYS:HG2	1.72	0.54
2:H:128:HIS:HD2	2:H:142:ARG:CZ	2.21	0.54
1:D:112:TRP:CE3	1:D:123:VAL:HG23	2.43	0.54
2:G:2:ARG:HA	2:G:17:CYS:HB2	1.89	0.53
2:E:96:ILE:HG13	2:E:178:GLU:HB3	1.89	0.53
2:E:184:LEU:HD22	2:E:216:ARG:HD2	1.91	0.53
2:G:273:HIS:CD2	2:G:274:PRO:HD2	2.44	0.53
1:B:93:GLN:HG2	2:G:273:HIS:CD2	2.44	0.53
2:G:223:LEU:HD23	2:G:242:ALA:CB	2.39	0.53
1:B:27:ASN:HB2	2:F:42:GLU:OE2	2.09	0.52
2:E:183:GLU:HA	2:E:183:GLU:OE2	2.09	0.52
2:E:220:ASN:OD1	2:E:221:GLN:NE2	2.42	0.52
2:F:183:GLU:OE2	2:F:183:GLU:HA	2.10	0.52
2:F:55:LEU:HD23	2:F:56:SER:N	2.24	0.52
1:B:25:PHE:CB	1:B:28:ILE:HD11	2.39	0.52
2:E:29:VAL:HG23	2:E:66:LEU:HG	1.92	0.52
2:G:58:ARG:NH2	2:G:112:SER:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:96:ILE:HD13	2:H:110:HIS:CD2	2.39	0.52
1:B:110:ARG:CG	1:B:110:ARG:HH11	2.22	0.52
1:D:65:ASP:C	1:D:67:MET:H	2.14	0.52
1:A:25:PHE:CB	1:A:28:ILE:HD11	2.40	0.52
2:G:77:ASN:O	2:G:79:GLY:N	2.42	0.51
2:H:2:ARG:HA	2:H:17:CYS:HB2	1.91	0.51
2:H:77:ASN:O	2:H:79:GLY:N	2.43	0.51
1:C:54:ASN:HD21	1:C:56:HIS:HD2	1.59	0.51
1:C:41:HIS:HB2	1:C:43:GLU:HG3	1.92	0.51
2:F:96:ILE:HG13	2:F:178:GLU:HB3	1.91	0.51
2:G:197:CYS:HB3	2:G:210:THR:HG22	1.92	0.51
1:A:74:TRP:CE3	1:A:96:LEU:HD22	2.45	0.51
2:F:260:HIS:CE1	5:F:328:SO4:S	3.04	0.51
2:H:198:LYS:HG2	2:H:236:TYR:OH	2.11	0.51
2:F:254:ASP:C	2:F:256:PHE:H	2.14	0.51
1:A:44:ILE:HD13	1:A:101:TYR:HE2	1.76	0.51
2:E:137:ARG:CG	2:E:138:PRO:HD3	2.26	0.51
2:H:198:LYS:HG3	2:H:238:VAL:HG22	1.92	0.50
2:G:198:LYS:HG3	2:G:238:VAL:HG22	1.92	0.50
2:H:75:LEU:C	2:H:77:ASN:H	2.15	0.50
2:H:102:ASP:OD1	2:H:104:SER:OG	2.30	0.50
2:E:190:ASN:HD22	2:E:215:CYS:HB2	1.76	0.50
2:F:220:ASN:OD1	2:F:221:GLN:NE2	2.45	0.50
2:G:75:LEU:C	2:G:77:ASN:H	2.14	0.50
1:C:118:GLY:O	1:C:119:LEU:HB2	2.11	0.50
2:E:260:HIS:CE1	5:E:318:SO4:S	3.04	0.50
1:A:110:ARG:HH11	1:A:110:ARG:CG	2.24	0.50
1:B:23:LYS:HD2	2:F:255:ALA:HA	1.94	0.50
2:G:26:THR:O	2:G:68:GLU:HA	2.12	0.49
1:C:129:HIS:CG	1:C:130:ASP:H	2.31	0.49
1:B:127:MET:HA	1:B:127:MET:CE	2.43	0.49
1:B:74:TRP:CE3	1:B:96:LEU:HD22	2.47	0.49
2:E:197:CYS:CB	2:E:210:THR:HG22	2.40	0.49
1:A:65:ASP:HA	1:A:126:CYS:HA	1.95	0.49
2:H:73:LEU:HD23	2:H:73:LEU:H	1.76	0.49
2:H:218:PRO:O	2:H:243:THR:HG22	2.13	0.49
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.76	0.49
1:D:76:SER:O	1:D:80:LEU:HG	2.13	0.49
1:D:23:LYS:HE3	2:H:127:THR:OG1	2.12	0.49
2:G:142:ARG:HG3	2:G:143:HIS:HD2	1.78	0.49
2:G:174:THR:C	2:G:176:CYS:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ARG:HD2	1:C:112:TRP:CD1	2.48	0.49
2:E:24:CYS:HA	2:E:45:CYS:HA	1.95	0.49
1:C:54:ASN:HD22	1:C:54:ASN:N	2.05	0.48
2:H:98:CYS:HB3	2:H:110:HIS:HB3	1.95	0.48
1:A:28:ILE:HD12	1:A:28:ILE:O	2.13	0.48
2:F:75:LEU:C	2:F:77:ASN:H	2.17	0.48
2:H:58:ARG:NH2	2:H:112:SER:O	2.44	0.48
2:F:160:HIS:HA	2:F:164:THR:O	2.13	0.48
2:G:255:ALA:C	2:G:257:SER:H	2.16	0.48
1:B:75:ASN:HD22	1:B:98:LYS:HG2	1.74	0.48
2:H:197:CYS:HB3	2:H:210:THR:HG22	1.95	0.48
1:A:112:TRP:CE3	1:A:123:VAL:HG13	2.48	0.48
1:B:76:SER:HB2	1:B:79:VAL:H	1.79	0.48
2:G:128:HIS:HD2	2:G:142:ARG:CZ	2.26	0.48
2:E:25:ARG:HB3	2:E:70:VAL:HG12	1.95	0.48
1:B:28:ILE:HD12	1:B:28:ILE:O	2.13	0.48
1:D:108:ARG:HD2	1:D:112:TRP:CD1	2.49	0.48
1:D:129:HIS:CG	1:D:130:ASP:H	2.31	0.48
1:B:11:CYS:SG	2:F:138:PRO:HG3	2.54	0.48
2:E:224:VAL:HG13	2:E:264:SER:HB3	1.96	0.48
2:G:142:ARG:HG3	2:G:143:HIS:CD2	2.49	0.48
2:F:251:HIS:H	2:F:252:LEU:HG	1.78	0.48
2:E:160:HIS:CD2	2:E:241:CYS:HB2	2.48	0.48
1:B:64:THR:HG22	6:B:154:HOH:O	2.14	0.48
2:G:98:CYS:HB3	2:G:110:HIS:HB3	1.96	0.47
2:H:18:ALA:O	2:H:20:GLY:N	2.46	0.47
2:H:26:THR:O	2:H:68:GLU:HA	2.13	0.47
1:C:65:ASP:C	1:C:67:MET:H	2.17	0.47
2:F:160:HIS:CE1	2:F:241:CYS:HB2	2.49	0.47
1:C:104:ASN:HD22	1:C:112:TRP:HE1	1.62	0.47
1:A:73:PRO:HD2	1:A:76:SER:OG	2.14	0.47
2:F:1:LEU:HD23	2:F:2:ARG:N	2.29	0.47
2:H:229:HIS:CD2	2:H:230:GLU:H	2.32	0.47
2:G:157:ASN:ND2	2:G:252:LEU:HD23	2.28	0.47
2:G:198:LYS:HG2	2:G:236:TYR:OH	2.15	0.47
1:D:80:LEU:HD23	1:D:85:HIS:HB2	1.97	0.47
2:E:75:LEU:C	2:E:77:ASN:H	2.18	0.47
2:G:73:LEU:H	2:G:73:LEU:HD23	1.79	0.47
1:B:65:ASP:HA	1:B:126:CYS:HA	1.97	0.47
1:C:59:ARG:HA	1:C:103:ARG:CZ	2.44	0.47
1:D:54:ASN:N	1:D:54:ASN:HD22	2.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:197:CYS:CB	2:F:210:THR:HG22	2.41	0.47
2:E:160:HIS:HA	2:E:164:THR:O	2.15	0.47
2:E:254:ASP:C	2:E:256:PHE:H	2.18	0.47
1:D:57:PHE:CD2	2:G:189:GLN:HG3	2.50	0.47
2:H:162:GLN:NE2	2:H:213:ILE:HD11	2.30	0.47
2:H:255:ALA:C	2:H:257:SER:H	2.18	0.47
2:F:5:GLN:O	2:F:12:CYS:HA	2.15	0.47
2:G:30:ARG:HB3	2:G:65:SER:HB2	1.97	0.47
2:H:174:THR:C	2:H:176:CYS:N	2.69	0.46
1:C:44:ILE:O	1:C:46:LYS:N	2.48	0.46
2:H:276:LEU:O	2:H:277:ASP:HB2	2.16	0.46
1:A:110:ARG:HH11	1:A:110:ARG:HG2	1.80	0.46
2:G:18:ALA:O	2:G:20:GLY:N	2.48	0.46
2:E:251:HIS:H	2:E:252:LEU:HG	1.80	0.46
2:E:5:GLN:O	2:E:12:CYS:HA	2.15	0.46
2:F:184:LEU:HD23	2:F:187:LEU:HD12	1.98	0.46
1:C:57:PHE:CD2	2:H:189:GLN:HG3	2.50	0.46
1:B:74:TRP:CD2	1:B:96:LEU:HD22	2.50	0.46
1:C:23:LYS:HE3	2:G:127:THR:OG1	2.15	0.46
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.63	0.46
2:G:130:ILE:HD12	2:G:130:ILE:HA	1.87	0.46
2:E:23:LEU:O	2:E:46:THR:N	2.49	0.46
2:E:130:ILE:HG21	2:E:166:HIS:CE1	2.51	0.46
2:G:128:HIS:HB2	2:G:142:ARG:NH2	2.31	0.46
2:E:153:CYS:HA	2:E:154:PRO:HA	1.68	0.46
1:D:26:SER:O	1:D:27:ASN:HB3	2.16	0.45
2:G:130:ILE:CG2	2:G:166:HIS:HE1	2.29	0.45
1:D:26:SER:O	1:D:27:ASN:CB	2.64	0.45
2:H:30:ARG:HB3	2:H:65:SER:HB2	1.97	0.45
2:E:1:LEU:HD23	2:E:2:ARG:N	2.32	0.45
1:B:120:LYS:HA	1:B:121:PRO:HD3	1.76	0.45
2:H:273:HIS:CD2	2:H:274:PRO:HD2	2.51	0.45
1:C:130:ASP:O	1:C:132:ALA:N	2.48	0.45
2:H:43:LYS:O	2:H:44:SER:HB3	2.17	0.45
2:G:206:SER:OG	2:G:209:GLU:OE2	2.34	0.45
1:A:127:MET:CE	1:A:127:MET:HA	2.45	0.45
2:E:55:LEU:HD23	2:E:56:SER:N	2.31	0.45
1:A:74:TRP:CD2	1:A:96:LEU:HD22	2.51	0.45
1:A:38:GLY:O	1:A:42:CYS:HA	2.16	0.45
2:H:157:ASN:HB3	2:H:244:ALA:HB3	1.99	0.45
1:A:130:ASP:C	1:A:132:ALA:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:99:GLY:N	2:G:104:SER:HB2	2.26	0.45
2:E:28:ILE:HB	2:E:67:THR:HG23	1.99	0.45
2:H:46:THR:OG1	2:H:50:LYS:HG3	2.17	0.45
2:F:28:ILE:HB	2:F:67:THR:HG23	1.99	0.44
2:F:190:ASN:HD22	2:F:215:CYS:HB2	1.81	0.44
2:H:142:ARG:HG3	2:H:143:HIS:CD2	2.52	0.44
2:H:219:MET:HG3	2:H:243:THR:HG23	1.99	0.44
2:H:157:ASN:ND2	2:H:252:LEU:HD23	2.32	0.44
2:G:190:ASN:HD22	2:G:192:ARG:H	1.66	0.44
1:B:72:LEU:HA	1:B:72:LEU:HD23	1.59	0.44
1:A:76:SER:HB2	1:A:79:VAL:H	1.82	0.44
2:E:5:GLN:HG3	2:E:15:GLU:HB2	1.99	0.44
2:F:190:ASN:HD22	2:F:192:ARG:HB3	1.81	0.44
1:D:130:ASP:O	1:D:132:ALA:N	2.50	0.44
2:E:150:LEU:HB3	2:E:151:PRO:HD2	2.00	0.44
1:C:109:ARG:NH2	1:C:109:ARG:HG3	2.31	0.44
1:A:30:TRP:CH2	2:E:66:LEU:HD21	2.52	0.44
2:E:184:LEU:HD23	2:E:187:LEU:HD12	2.00	0.44
1:A:23:LYS:N	2:E:140:ASP:OD1	2.49	0.44
2:G:102:ASP:OD1	2:G:104:SER:OG	2.35	0.44
1:D:44:ILE:O	1:D:46:LYS:N	2.51	0.44
2:E:263:VAL:CG1	2:E:264:SER:N	2.67	0.44
1:B:73:PRO:HA	1:B:99:HIS:O	2.18	0.44
2:E:260:HIS:HE1	5:E:318:SO4:O3	1.98	0.44
2:H:190:ASN:HD22	2:H:192:ARG:H	1.65	0.44
2:H:206:SER:OG	2:H:209:GLU:OE2	2.36	0.44
2:H:142:ARG:HG3	2:H:143:HIS:HD2	1.83	0.43
2:H:99:GLY:N	2:H:104:SER:HB2	2.31	0.43
2:H:190:ASN:ND2	2:H:192:ARG:HB3	2.33	0.43
2:G:261:ILE:HG12	2:G:262:ASP:N	2.34	0.43
2:G:178:GLU:HG2	2:G:179:GLY:N	2.34	0.43
1:D:73:PRO:HA	1:D:99:HIS:O	2.19	0.43
2:E:189:GLN:HE21	2:E:189:GLN:CA	2.29	0.43
2:F:25:ARG:NH1	2:F:27:THR:OG1	2.46	0.43
2:E:25:ARG:NH1	2:E:27:THR:OG1	2.46	0.43
2:F:126:VAL:HG11	2:F:165:PHE:CE2	2.53	0.43
1:B:130:ASP:C	1:B:132:ALA:N	2.71	0.43
2:G:174:THR:C	2:G:176:CYS:H	2.22	0.43
2:F:206:SER:HG	2:F:209:GLU:HG3	1.83	0.43
1:C:80:LEU:HD23	1:C:85:HIS:HB2	2.00	0.43
2:H:160:HIS:CE1	2:H:241:CYS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:142:ARG:NH1	2:G:183:GLU:OE2	2.52	0.43
2:G:60:GLY:O	2:G:61:LEU:HB2	2.18	0.43
2:G:218:PRO:O	2:G:243:THR:HG22	2.18	0.43
2:E:192:ARG:HG3	2:E:193:GLN:N	2.34	0.42
2:H:128:HIS:CE1	2:H:129:TRP:HB2	2.54	0.42
2:H:128:HIS:CD2	2:H:142:ARG:CZ	3.01	0.42
2:H:261:ILE:HG12	2:H:262:ASP:N	2.34	0.42
2:E:126:VAL:HG11	2:E:165:PHE:CE2	2.54	0.42
2:H:130:ILE:CG2	2:H:166:HIS:HE1	2.29	0.42
2:F:159:PHE:CE2	2:F:256:PHE:HZ	2.37	0.42
2:G:187:LEU:HA	2:G:188:PRO:HD2	1.89	0.42
2:F:224:VAL:HG13	2:F:264:SER:HB3	2.01	0.42
2:H:60:GLY:O	2:H:61:LEU:HB2	2.20	0.42
2:F:24:CYS:HA	2:F:45:CYS:HA	2.01	0.42
2:G:213:ILE:HD12	2:G:213:ILE:HA	1.90	0.42
2:G:100:SER:CB	2:G:142:ARG:HB3	2.49	0.42
1:C:75:ASN:HD22	1:C:98:LYS:HG2	1.84	0.42
1:A:54:ASN:N	1:A:54:ASN:HD22	2.08	0.42
2:H:58:ARG:HG3	2:H:113:LEU:HD13	2.01	0.42
2:F:256:PHE:O	2:F:257:SER:C	2.58	0.42
1:C:26:SER:O	1:C:27:ASN:CB	2.67	0.42
1:C:26:SER:O	1:C:27:ASN:HB3	2.20	0.42
1:C:109:ARG:NH2	1:C:109:ARG:CG	2.80	0.42
2:H:178:GLU:HG2	2:H:179:GLY:N	2.35	0.42
1:D:54:ASN:H	1:D:54:ASN:ND2	2.08	0.42
1:B:127:MET:HA	1:B:127:MET:HE3	2.02	0.42
1:D:75:ASN:HD22	1:D:98:LYS:HG2	1.85	0.42
1:D:106:ASP:N	1:D:106:ASP:OD2	2.53	0.42
1:D:20:VAL:HG12	1:D:21:SER:N	2.35	0.42
2:H:276:LEU:O	2:H:277:ASP:CB	2.68	0.42
1:A:23:LYS:HD2	2:E:255:ALA:HA	2.02	0.42
2:F:139:LYS:HB3	2:F:139:LYS:HE2	1.83	0.42
2:H:100:SER:CB	2:H:142:ARG:HB3	2.50	0.41
2:G:197:CYS:CB	2:G:210:THR:HG22	2.50	0.41
2:H:213:ILE:HA	2:H:213:ILE:HD12	1.89	0.41
2:F:239:ARG:NH2	2:F:274:PRO:HA	2.35	0.41
1:B:73:PRO:HD2	1:B:76:SER:OG	2.19	0.41
2:G:190:ASN:C	2:G:190:ASN:HD22	2.22	0.41
2:F:153:CYS:HA	2:F:154:PRO:HA	1.65	0.41
2:E:256:PHE:O	2:E:257:SER:C	2.58	0.41
2:G:190:ASN:ND2	2:G:192:ARG:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:190:ASN:HD21	2:G:192:ARG:HB3	1.86	0.41
2:G:229:HIS:CD2	2:G:230:GLU:H	2.38	0.41
2:G:1:LEU:HD23	2:G:2:ARG:N	2.35	0.41
2:G:75:LEU:O	2:G:77:ASN:N	2.54	0.41
2:H:198:LYS:HA	2:H:237:MET:O	2.21	0.41
2:G:47:HIS:CE1	2:G:233:GLN:OE1	2.74	0.41
2:F:259:ASN:O	2:F:260:HIS:C	2.58	0.41
1:A:109:ARG:HG3	1:A:110:ARG:HG2	2.03	0.41
1:A:130:ASP:C	1:A:132:ALA:H	2.24	0.41
2:H:31:LEU:HA	2:H:63:ILE:O	2.21	0.41
2:H:58:ARG:HG2	2:H:63:ILE:HG13	2.03	0.41
1:A:73:PRO:O	1:A:76:SER:OG	2.29	0.41
2:G:128:HIS:CE1	2:G:129:TRP:HB2	2.54	0.41
1:D:32:ASN:HA	1:D:32:ASN:HD22	1.55	0.41
2:H:97:SER:N	2:H:111:GLN:O	2.51	0.41
1:D:59:ARG:HA	1:D:103:ARG:CZ	2.51	0.41
2:F:137:ARG:CG	2:F:138:PRO:HD3	2.32	0.40
1:D:109:ARG:HG3	1:D:109:ARG:NH2	2.34	0.40
1:D:65:ASP:OD2	1:D:67:MET:HB2	2.21	0.40
2:H:160:HIS:CD2	2:H:184:LEU:HD11	2.56	0.40
2:F:275:ASP:C	2:F:277:ASP:H	2.23	0.40
2:F:273:HIS:ND1	2:F:274:PRO:CD	2.84	0.40
2:E:173:THR:HB	2:E:176:CYS:HB3	2.03	0.40
2:F:23:LEU:O	2:F:46:THR:N	2.53	0.40
1:B:23:LYS:N	2:F:140:ASP:OD1	2.51	0.40
2:E:198:LYS:O	2:E:205:CYS:SG	2.80	0.40
2:G:31:LEU:HA	2:G:63:ILE:O	2.21	0.40
2:F:256:PHE:HB3	2:F:258:MET:HG3	2.04	0.40
1:B:85:HIS:CE1	1:B:88:ARG:HG3	2.57	0.40
2:F:229:HIS:CD2	2:F:230:GLU:N	2.89	0.40
2:E:206:SER:O	2:E:210:THR:HG23	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	120/145 (83%)	109 (91%)	9 (8%)	2 (2%)	11	36
1	B	120/145 (83%)	108 (90%)	11 (9%)	1 (1%)	24	58
1	C	120/145 (83%)	94 (78%)	18 (15%)	8 (7%)	1	4
1	D	120/145 (83%)	98 (82%)	16 (13%)	6 (5%)	3	8
2	E	257/279 (92%)	209 (81%)	37 (14%)	11 (4%)	3	10
2	F	257/279 (92%)	208 (81%)	37 (14%)	12 (5%)	3	9
2	G	236/279 (85%)	194 (82%)	22 (9%)	20 (8%)	1	2
2	H	236/279 (85%)	196 (83%)	21 (9%)	19 (8%)	1	2
All	All	1466/1696 (86%)	1216 (83%)	171 (12%)	79 (5%)	2	7

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	119	LEU
1	D	119	LEU
2	E	36	GLU
2	E	201	SER
2	F	36	GLU
2	F	201	SER
2	G	78	GLN
2	G	79	GLY
2	G	209	GLU
2	H	19	LEU
2	H	78	GLN
2	H	209	GLU
2	H	233	GLN
1	D	107	ASN
2	E	8	THR
2	E	60	GLY
2	E	79	GLY
2	E	185	GLU
2	F	60	GLY
2	F	79	GLY
2	F	185	GLU
2	G	19	LEU
2	G	73	LEU
2	G	76	CYS

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Mol	Chain	Res	Type
2	G	232	LYS
2	G	233	GLN
2	G	257	SER
2	H	73	LEU
2	H	75	LEU
2	H	76	CYS
2	H	79	GLY
2	H	173	THR
2	H	232	LYS
2	H	257	SER
1	C	91	ALA
1	C	107	ASN
1	C	131	CYS
2	E	1	LEU
2	E	34	GLU
2	E	80	ASN
2	E	256	PHE
2	F	8	THR
2	F	80	ASN
2	F	151	PRO
2	F	256	PHE
2	G	17	CYS
2	G	75	LEU
2	G	101	SER
2	G	173	THR
2	G	255	ALA
2	H	17	CYS
2	H	44	SER
2	H	101	SER
2	H	255	ALA
1	A	26	SER
1	C	116	GLN
1	D	26	SER
1	D	91	ALA
1	D	116	GLN
2	E	151	PRO
2	F	1	LEU
2	F	34	GLU
2	G	8	THR
2	G	20	GLY
2	G	44	SER
2	G	231	PRO

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Mol	Chain	Res	Type
2	H	20	GLY
2	H	231	PRO
1	B	26	SER
1	C	35	LYS
1	C	45	ASP
1	D	47	SER
2	F	13	ARG
2	G	60	GLY
2	H	60	GLY
1	C	47	SER
2	G	48	SER
2	H	48	SER
1	A	28	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	106/128 (83%)	99 (93%)	7 (7%)	21	51
1	B	106/128 (83%)	100 (94%)	6 (6%)	25	58
1	C	106/128 (83%)	99 (93%)	7 (7%)	21	51
1	D	106/128 (83%)	99 (93%)	7 (7%)	21	51
2	E	236/247 (96%)	212 (90%)	24 (10%)	9	26
2	F	236/247 (96%)	213 (90%)	23 (10%)	10	29
2	G	220/247 (89%)	203 (92%)	17 (8%)	16	41
2	H	220/247 (89%)	205 (93%)	15 (7%)	20	49
All	All	1336/1500 (89%)	1230 (92%)	106 (8%)	15	40

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	83	THR
1	A	110	ARG
1	A	120	LYS
1	A	127	MET
1	A	130	ASP
1	B	43	GLU
1	B	54	ASN
1	B	83	THR
1	B	110	ARG
1	B	120	LYS
1	B	127	MET
1	C	32	ASN
1	C	43	GLU
1	C	54	ASN
1	C	59	ARG
1	C	64	THR
1	C	109	ARG
1	C	127	MET
1	D	32	ASN
1	D	43	GLU
1	D	54	ASN
1	D	59	ARG
1	D	64	THR
1	D	109	ARG
1	D	127	MET
2	E	1	LEU
2	E	23	LEU
2	E	30	ARG
2	E	40	LEU
2	E	67	THR
2	E	77	ASN
2	E	80	ASN
2	E	110	HIS
2	E	116	ARG
2	E	119	GLU
2	E	151	PRO
2	E	171	CYS
2	E	182	LEU
2	E	184	LEU
2	E	189	GLN
2	E	192	ARG
2	E	208	GLU

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Mol	Chain	Res	Type
2	E	221	GLN
2	E	223	LEU
2	E	245	SER
2	E	252	LEU
2	E	259	ASN
2	E	261	ILE
2	E	277	ASP
2	F	1	LEU
2	F	23	LEU
2	F	40	LEU
2	F	67	THR
2	F	77	ASN
2	F	80	ASN
2	F	110	HIS
2	F	116	ARG
2	F	119	GLU
2	F	151	PRO
2	F	171	CYS
2	F	182	LEU
2	F	184	LEU
2	F	189	GLN
2	F	192	ARG
2	F	208	GLU
2	F	221	GLN
2	F	223	LEU
2	F	245	SER
2	F	252	LEU
2	F	259	ASN
2	F	261	ILE
2	F	277	ASP
2	G	17	CYS
2	G	29	VAL
2	G	54	THR
2	G	73	LEU
2	G	77	ASN
2	G	110	HIS
2	G	116	ARG
2	G	117	SER
2	G	162	GLN
2	G	164	THR
2	G	189	GLN
2	G	190	ASN

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Mol	Chain	Res	Type
2	G	221	GLN
2	G	223	LEU
2	G	226	THR
2	G	232	LYS
2	G	256	PHE
2	H	17	CYS
2	H	29	VAL
2	H	54	THR
2	H	73	LEU
2	H	77	ASN
2	H	110	HIS
2	H	117	SER
2	H	164	THR
2	H	189	GLN
2	H	190	ASN
2	H	221	GLN
2	H	223	LEU
2	H	226	THR
2	H	232	LYS
2	H	256	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	41	HIS
1	A	54	ASN
1	A	93	GLN
1	A	107	ASN
1	A	116	GLN
1	B	40	GLN
1	B	41	HIS
1	B	54	ASN
1	B	93	GLN
1	B	107	ASN
1	B	116	GLN
1	C	15	ASN
1	C	32	ASN
1	C	54	ASN
1	C	56	HIS
1	C	82	GLN
1	C	93	GLN

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Mol	Chain	Res	Type
1	C	104	ASN
1	D	15	ASN
1	D	54	ASN
1	D	56	HIS
1	D	82	GLN
1	D	93	GLN
1	D	104	ASN
2	E	77	ASN
2	E	78	GLN
2	E	80	ASN
2	E	111	GLN
2	E	121	GLN
2	E	128	HIS
2	E	189	GLN
2	E	190	ASN
2	E	193	GLN
2	E	221	GLN
2	E	233	GLN
2	E	259	ASN
2	F	77	ASN
2	F	78	GLN
2	F	80	ASN
2	F	111	GLN
2	F	121	GLN
2	F	128	HIS
2	F	160	HIS
2	F	189	GLN
2	F	190	ASN
2	F	193	GLN
2	F	221	GLN
2	F	233	GLN
2	F	259	ASN
2	G	21	GLN
2	G	78	GLN
2	G	80	ASN
2	G	110	HIS
2	G	111	GLN
2	G	114	GLN
2	G	128	HIS
2	G	131	GLN
2	G	160	HIS
2	G	162	GLN

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Mol	Chain	Res	Type
2	G	166	HIS
2	G	172	GLN
2	G	190	ASN
2	G	193	GLN
2	G	221	GLN
2	G	229	HIS
2	G	233	GLN
2	G	234	GLN
2	G	260	HIS
2	G	273	HIS
2	H	21	GLN
2	H	78	GLN
2	H	80	ASN
2	H	110	HIS
2	H	111	GLN
2	H	114	GLN
2	H	128	HIS
2	H	131	GLN
2	H	160	HIS
2	H	162	GLN
2	H	166	HIS
2	H	172	GLN
2	H	190	ASN
2	H	193	GLN
2	H	221	GLN
2	H	229	HIS
2	H	234	GLN
2	H	260	HIS
2	H	273	HIS

### 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 ⓘ

10 carbohydrates 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	$\# Z  > 2$
3	NAG	E	311	3,2	14,14,15	0.46	0	15,19,21	1.20	1 (6%)
3	NAG	E	312	3	14,14,15	0.41	0	15,19,21	2.09	2 (13%)
3	BMA	E	317	3	11,11,12	0.67	0	14,15,17	0.93	0
3	NAG	F	321	3,2	14,14,15	0.57	0	15,19,21	1.39	3 (20%)
3	NAG	F	322	3	14,14,15	0.49	0	15,19,21	1.96	2 (13%)
3	BMA	F	327	3	11,11,12	0.66	0	14,15,17	0.67	0
4	NAG	G	331	2,4	14,14,15	0.47	0	15,19,21	1.29	1 (6%)
4	NAG	G	332	4	14,14,15	0.49	0	15,19,21	1.88	4 (26%)
4	NAG	H	341	4	14,14,15	0.47	0	15,19,21	1.29	1 (6%)
4	NAG	H	342	4	14,14,15	0.54	0	15,19,21	1.82	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	311	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	312	3	-	0/6/23/26	0/1/1/1
3	BMA	E	317	3	-	0/2/19/22	0/1/1/1
3	NAG	F	321	3,2	-	0/6/23/26	0/1/1/1
3	NAG	F	322	3	-	0/6/23/26	0/1/1/1
3	BMA	F	327	3	-	0/2/19/22	0/1/1/1
4	NAG	G	331	2,4	-	0/6/23/26	0/1/1/1
4	NAG	G	332	4	-	0/6/23/26	0/1/1/1
4	NAG	H	341	4	-	0/6/23/26	0/1/1/1
4	NAG	H	342	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	322	NAG	C4-C3-C2	-4.80	103.77	111.23
3	E	312	NAG	C4-C3-C2	-4.03	104.97	111.23
3	F	321	NAG	O4-C4-C3	-2.58	104.53	110.34
3	F	321	NAG	O3-C3-C4	-2.03	105.76	110.34
4	G	332	NAG	O5-C5-C6	2.01	111.70	107.35
3	F	321	NAG	C1-O5-C5	2.06	114.86	112.25
4	G	332	NAG	C2-N2-C7	2.21	125.88	123.04
4	G	332	NAG	C3-C4-C5	2.41	114.40	110.20
3	E	311	NAG	C3-C2-N2	2.43	116.39	110.56
4	H	341	NAG	C1-O5-C5	3.17	116.27	112.25
4	G	331	NAG	O5-C5-C6	3.18	114.23	107.35
3	F	322	NAG	C1-O5-C5	4.45	117.90	112.25
4	G	332	NAG	C1-O5-C5	5.90	119.73	112.25
3	E	312	NAG	C1-O5-C5	5.90	119.73	112.25
4	H	342	NAG	C1-O5-C5	6.36	120.32	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	342	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	311	NAG	1	0
3	E	312	NAG	1	0
3	F	321	NAG	1	0
3	F	322	NAG	1	0
4	H	341	NAG	1	0

## 5.6 Ligand geometry [i](#)

2 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
5	SO4	E	318	-	4,4,4	0.34	0	6,6,6	1.10	1 (16%)
5	SO4	F	328	-	4,4,4	0.48	0	6,6,6	0.60	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
5	SO4	E	318	-	-	0/0/0/0	0/0/0/0
5	SO4	F	328	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	318	SO4	O2-S-O1	-2.03	103.06	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	318	SO4	4	0
5	F	328	SO4	3	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	122/145 (84%)	-0.30	0	100	100	50, 65, 80, 92	0
1	B	122/145 (84%)	-0.28	0	100	100	50, 65, 80, 92	0
1	C	122/145 (84%)	0.24	8 (6%)	22	13	49, 67, 77, 80	0
1	D	122/145 (84%)	0.24	7 (5%)	27	17	49, 67, 76, 80	0
2	E	265/279 (94%)	0.13	13 (4%)	33	22	48, 70, 91, 104	0
2	F	265/279 (94%)	0.15	15 (5%)	27	17	48, 70, 91, 104	0
2	G	248/279 (88%)	0.48	29 (11%)	6	3	48, 68, 80, 92	0
2	H	248/279 (88%)	0.48	26 (10%)	8	4	48, 68, 80, 92	0
All	All	1514/1696 (89%)	0.20	98 (6%)	22	13	48, 68, 85, 104	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	131	GLN	6.7
2	E	131	GLN	6.7
2	G	19	LEU	6.5
2	H	19	LEU	5.9
2	H	173	THR	5.2
2	G	131	GLN	5.1
2	H	131	GLN	5.1
1	C	127	MET	4.7
2	G	251	HIS	4.6
2	F	81	SER	4.6
1	D	127	MET	4.3
2	H	1	LEU	4.2
2	G	173	THR	4.2
2	E	81	SER	4.1
2	F	83	ARG	4.1
2	H	251	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	66	THR	3.9
2	G	1	LEU	3.8
2	G	61	LEU	3.8
2	H	232	LYS	3.6
2	E	83	ARG	3.6
2	F	233	GLN	3.6
2	E	32	TRP	3.5
2	G	232	LYS	3.4
2	H	61	LEU	3.4
2	G	116	ARG	3.4
1	C	66	THR	3.4
1	C	129	HIS	3.4
2	G	231	PRO	3.4
2	F	235	SER	3.4
2	H	118	PRO	3.3
2	H	18	ALA	3.2
1	D	129	HIS	3.2
2	E	0	SER	3.2
2	E	235	SER	3.1
2	G	18	ALA	3.1
2	H	231	PRO	3.1
2	E	233	GLN	3.1
2	F	32	TRP	3.0
2	H	116	ARG	3.0
1	C	64	THR	3.0
2	G	260	HIS	3.0
2	H	10	GLY	2.9
2	G	118	PRO	2.9
2	G	230	GLU	2.9
2	G	10	GLY	2.9
2	E	80	ASN	2.9
1	D	11	CYS	2.8
2	E	137	ARG	2.8
2	H	234	GLN	2.7
2	H	174	THR	2.7
2	G	114	GLN	2.7
2	F	251	HIS	2.6
1	C	119	LEU	2.6
2	F	137	ARG	2.6
2	F	82	GLY	2.6
2	E	79	GLY	2.6
2	G	2	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	260	HIS	2.5
2	G	82	GLY	2.5
2	G	81	SER	2.5
2	F	203	HIS	2.5
2	G	97	SER	2.5
2	G	110	HIS	2.5
2	H	114	GLN	2.5
2	E	19	LEU	2.5
2	H	222	CYS	2.5
2	H	230	GLU	2.5
1	D	126	CYS	2.5
2	H	103	MET	2.5
1	C	126	CYS	2.4
2	H	97	SER	2.4
2	H	2	ARG	2.4
1	D	70	PRO	2.4
1	C	70	PRO	2.4
2	H	110	HIS	2.3
2	E	82	GLY	2.3
2	F	19	LEU	2.3
2	G	63	ILE	2.3
2	H	233	GLN	2.3
2	G	36	GLU	2.3
2	F	0	SER	2.2
2	G	172	GLN	2.2
2	G	203	HIS	2.2
2	F	91	ARG	2.2
2	E	232	LYS	2.2
1	C	67	MET	2.2
2	G	233	GLN	2.2
1	D	119	LEU	2.1
2	H	81	SER	2.1
2	G	222	CYS	2.1
2	G	80	ASN	2.1
2	H	235	SER	2.1
2	G	234	GLN	2.0
2	F	116	ARG	2.0
2	H	203	HIS	2.0
2	G	21	GLN	2.0
2	F	80	ASN	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](#)

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
4	NAG	G	332	14/15	0.85	0.35	-	94,129,153,156	0
3	BMA	F	327	11/12	0.72	0.26	-	97,155,174,194	0
3	NAG	E	311	14/15	0.96	0.26	-	66,91,107,116	0
3	BMA	E	317	11/12	0.71	0.25	-	107,159,168,181	0
3	NAG	F	322	14/15	0.84	0.28	-	55,99,125,152	0
3	NAG	E	312	14/15	0.86	0.25	-	73,96,142,161	0
3	NAG	F	321	14/15	0.96	0.28	-	58,83,112,116	0
4	NAG	H	342	14/15	0.85	0.33	-	85,138,149,150	0
4	NAG	H	341	14/15	0.49	0.28	-	80,164,186,192	0
4	NAG	G	331	14/15	0.72	0.25	-	80,138,160,163	0

## 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
5	SO4	E	318	5/5	0.99	0.09	-1.56	52,57,75,81	0
5	SO4	F	328	5/5	0.98	0.08	-1.59	54,56,74,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.