Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:19 PM GMT

PDB ID	:	4EEF
Title	:	Crystal structure of the designed inhibitor protein F-HB80.4 in complex with the 1918 influenza virus hemagglutinin.
Authors	:	Dreyfus, C.; Wilson, I.A.
Deposited on	:	2012-03-28
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

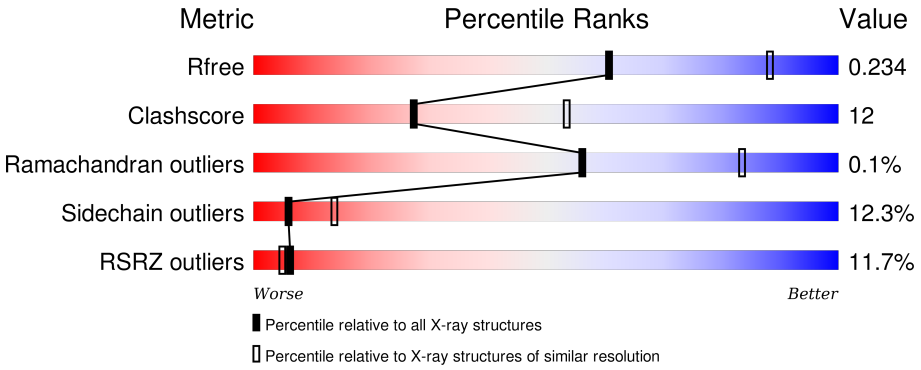
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	331	3% 74% 21%
1	C	331	% 73% 22%
1	E	331	2% 69% 25%
2	B	179	22% 61% 29% 6%
2	D	179	16% 61% 32%

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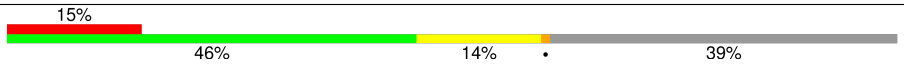
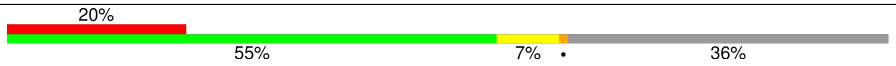
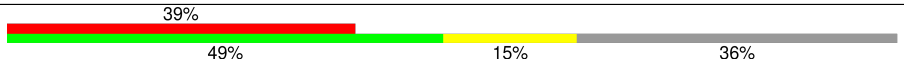
Mol	Chain	Length	Quality of chain
2	F	179	
3	G	74	
3	H	74	
3	I	74	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12880 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	8	2	0
			2529	1594	434	490	11			
1	C	323	Total	C	N	O	S	6	1	0
			2510	1583	431	485	11			
1	E	323	Total	C	N	O	S	0	1	0
			2512	1583	432	486	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	THR	CONFLICT	UNP Q9WFX3
A	9	PRO	ASN	CONFLICT	UNP Q9WFX3
A	10	GLY	ALA	CONFLICT	UNP Q9WFX3
C	8	ASP	THR	CONFLICT	UNP Q9WFX3
C	9	PRO	ASN	CONFLICT	UNP Q9WFX3
C	10	GLY	ALA	CONFLICT	UNP Q9WFX3
E	8	ASP	THR	CONFLICT	UNP Q9WFX3
E	9	PRO	ASN	CONFLICT	UNP Q9WFX3
E	10	GLY	ALA	CONFLICT	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1394	871	239	278	6			
2	D	173	Total	C	N	O	S	5	1	0
			1399	874	240	279	6			
2	F	171	Total	C	N	O	S	0	1	0
			1382	863	238	275	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	EXPRESSION TAG	UNP Q9WFX3
B	178	GLY	-	EXPRESSION TAG	UNP Q9WFX3
B	179	ARG	-	EXPRESSION TAG	UNP Q9WFX3
D	177	SER	-	EXPRESSION TAG	UNP Q9WFX3
D	178	GLY	-	EXPRESSION TAG	UNP Q9WFX3
D	179	ARG	-	EXPRESSION TAG	UNP Q9WFX3
F	177	SER	-	EXPRESSION TAG	UNP Q9WFX3
F	178	GLY	-	EXPRESSION TAG	UNP Q9WFX3
F	179	ARG	-	EXPRESSION TAG	UNP Q9WFX3

- Molecule 3 is a protein called F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	45	Total	C	N	O	0	0	0
			301	195	49	57			
3	H	47	Total	C	N	O	0	0	0
			303	195	53	55			
3	I	47	Total	C	N	O	0	0	0
			294	187	53	54			

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	13	Total	O	0	0
			13	13		
5	C	37	Total	O	0	0
			37	37		
5	D	7	Total	O	0	0
			7	7		

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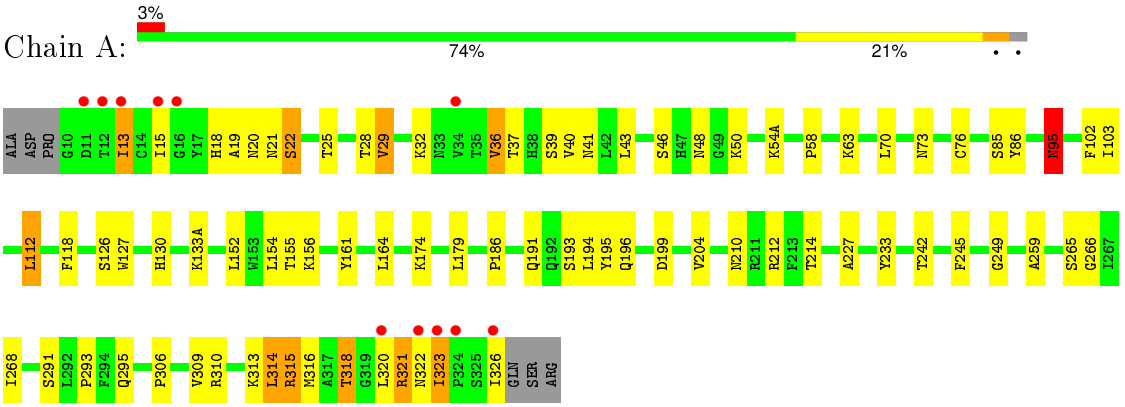
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	23	Total O 23 23	0	0
5	F	9	Total O 9 9	0	0

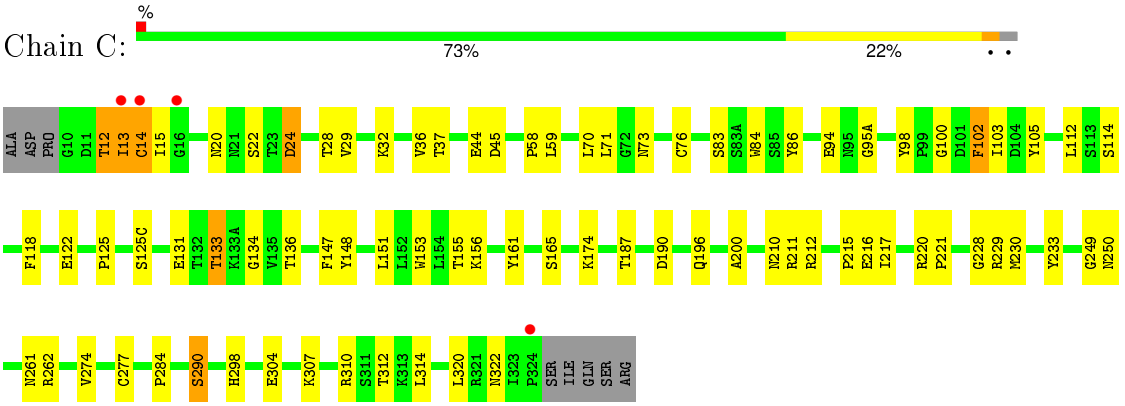
3 Residue-property plots (i)

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.

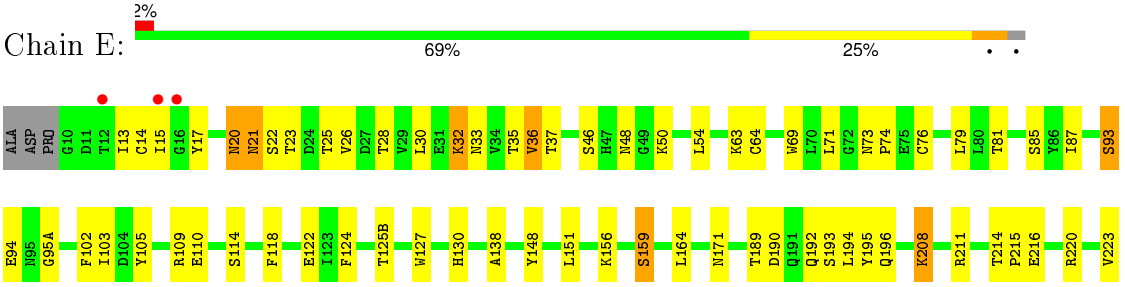
- Molecule 1: Hemagglutinin HA1 chain

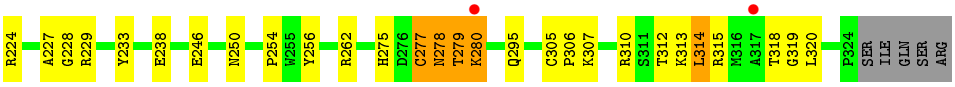


- Molecule 1: Hemagglutinin HA1 chain



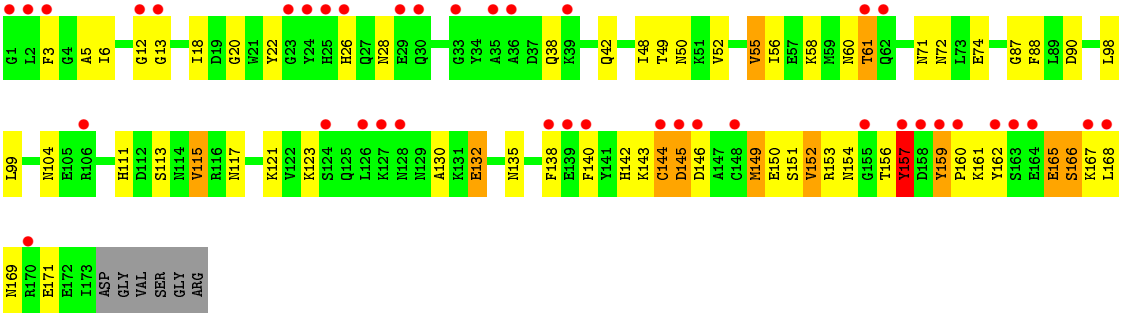
- Molecule 1: Hemagglutinin HA1 chain





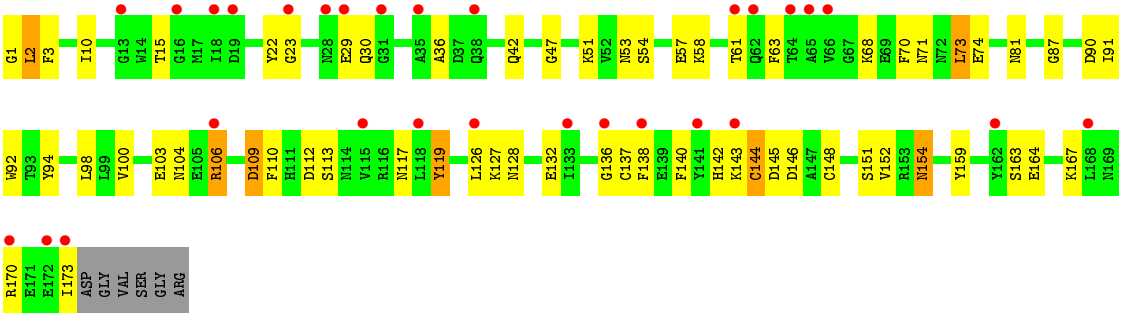
• Molecule 2: Hemagglutinin HA2 chain

Chain B:



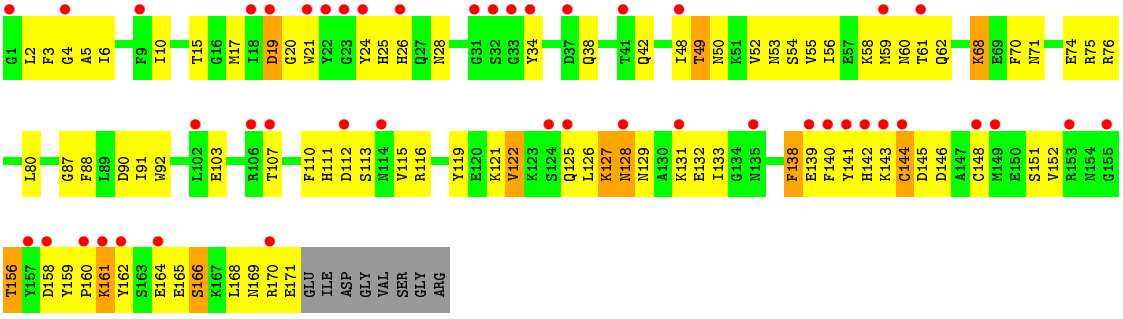
• Molecule 2: Hemagglutinin HA2 chain

Chain D:



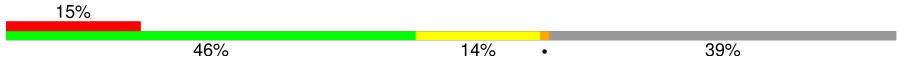
• Molecule 2: Hemagglutinin HA2 chain

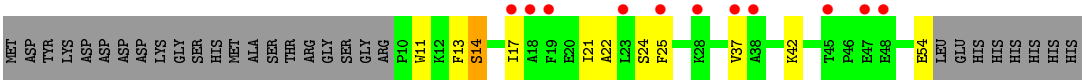
Chain F:



• Molecule 3: F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN

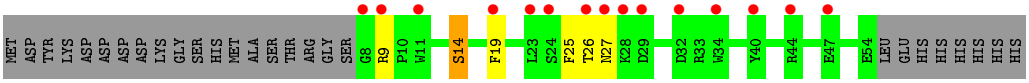
Chain G:





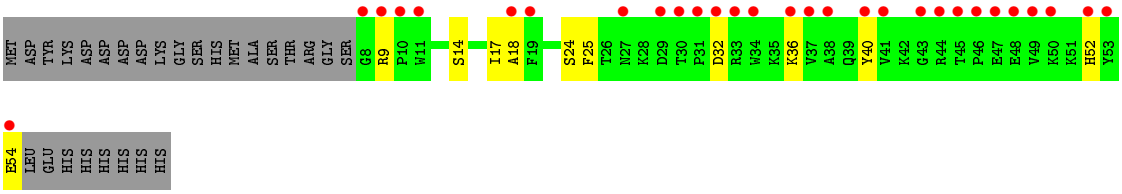
• Molecule 3: F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN

Chain H:



• Molecule 3: F-HB80.4, DESIGNED HEMAGGLUTININ BINDING PROTEIN

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.33Å 126.15Å 243.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.67 – 2.70 43.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.1 (43.67-2.70) 90.2 (43.67-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.43 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.229 , 0.285 0.228 , 0.234	Depositor DCC
R_{free} test set	2846 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	58.7	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 61.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 58127 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12880	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.50	0/2596	0.67	0/3536
1	C	0.50	0/2577	0.66	0/3510
1	E	0.48	0/2576	0.64	0/3509
2	B	0.42	0/1421	0.65	1/1913 (0.1%)
2	D	0.39	0/1429	0.58	0/1924
2	F	0.38	0/1412	0.61	0/1901
3	G	0.38	0/308	0.63	0/421
3	H	0.30	0/309	0.60	0/423
3	I	0.29	0/299	0.54	0/409
All	All	0.45	0/12927	0.64	1/17546 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	F	0	2
3	G	0	1
3	H	0	3
3	I	0	1
All	All	0	9

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	149	MET	CG-SD-CE	6.58	110.73	100.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	ASN	Peptide
2	B	157	TYR	Peptide
2	F	144	CYS	Peptide
2	F	168	LEU	Peptide
3	G	42	LYS	Peptide
3	H	25	PHE	Peptide
3	H	27	ASN	Peptide
3	H	9	ARG	Peptide
3	I	9	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2529	0	2453	46	0
1	C	2510	0	2435	52	0
1	E	2512	0	2431	71	0
2	B	1394	0	1312	59	0
2	D	1399	0	1318	51	0
2	F	1382	0	1300	75	0
3	G	301	0	212	9	0
3	H	303	0	217	1	0
3	I	294	0	203	8	0
4	A	39	0	34	0	0
4	C	39	0	34	0	0
4	E	39	0	34	1	0
5	A	50	0	0	0	0
5	B	13	0	0	0	0
5	C	37	0	0	1	0
5	D	7	0	0	0	0
5	E	23	0	0	2	0
5	F	9	0	0	1	0
All	All	12880	0	11983	294	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 12.

All (294) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:LYS:HD2	2:F:59:MET:CE	1.70	1.19
1:E:307:LYS:CD	2:F:59:MET:CE	2.25	1.13
1:E:307:LYS:HD2	2:F:59:MET:HE3	1.12	1.10
3:G:14:SER:HA	3:G:17:ILE:HD12	1.32	1.10
2:D:70:PHE:HA	2:D:74:GLU:OE1	1.51	1.10
1:E:307:LYS:HD3	2:F:59:MET:HE1	1.30	1.07
1:E:307:LYS:CD	2:F:59:MET:HE1	1.86	1.05
1:E:307:LYS:CD	2:F:59:MET:HE3	1.95	0.93
2:B:49:THR:HG22	3:G:17:ILE:HG22	1.48	0.93
2:D:70:PHE:CA	2:D:74:GLU:OE1	2.17	0.92
1:A:13:ILE:HG13	2:B:149:MET:HE2	1.60	0.83
2:F:71:ASN:OD1	2:F:74:GLU:HG3	1.82	0.80
1:A:13:ILE:HB	2:B:26:HIS:HD2	1.45	0.80
1:C:70:LEU:HD11	1:C:112:LEU:HD11	1.65	0.79
1:A:323:ILE:HG12	2:B:13:GLY:H	1.47	0.78
2:B:49:THR:HG22	3:G:17:ILE:CG2	2.14	0.77
1:C:13:ILE:HD11	2:D:126:LEU:HD11	1.66	0.77
3:G:14:SER:O	3:G:17:ILE:HB	1.86	0.76
2:F:151:SER:OG	2:F:156:THR:O	2.04	0.76
2:D:2:LEU:HD22	2:D:109:ASP:HB2	1.67	0.75
3:G:14:SER:HA	3:G:17:ILE:CD1	2.16	0.75
2:D:71:ASN:OD1	2:D:74:GLU:HG3	1.87	0.75
1:E:307:LYS:HD3	2:F:59:MET:CE	2.01	0.75
2:F:17:MET:HG2	2:F:34:TYR:HB3	1.67	0.75
2:B:123:LYS:NZ	2:B:132:GLU:OE1	2.20	0.74
2:D:71:ASN:N	2:D:74:GLU:OE1	2.20	0.74
2:F:70:PHE:HA	2:F:74:GLU:OE1	1.88	0.73
1:C:187:THR:OG1	1:C:190:ASP:OD2	2.06	0.72
2:D:113:SER:OG	2:F:2:LEU:O	2.07	0.72
1:A:212:ARG:NH1	1:C:217:ILE:O	2.24	0.71
1:E:76:CYS:HB3	1:E:79:LEU:HD12	1.72	0.71
1:E:307:LYS:HE2	2:F:92:TRP:CD2	2.26	0.71
1:A:70:LEU:HD11	1:A:112:LEU:HD21	1.72	0.70
1:E:138:ALA:O	1:E:224:ARG:NH1	2.25	0.70
1:C:174:LYS:NZ	1:C:261:ASN:HD21	1.90	0.70
2:B:154:ASN:HB3	2:B:156:THR:HG23	1.74	0.69
2:D:91:ILE:HD12	2:D:92:TRP:N	2.08	0.69
2:F:142:HIS:NE2	2:F:162:TYR:O	2.25	0.69
2:D:71:ASN:H	2:D:74:GLU:CD	1.95	0.69
1:C:114:SER:HB3	1:C:262:ARG:HH11	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ARG:NH1	2:D:90:ASP:OD1	2.26	0.68
2:F:119:TYR:OH	2:F:132:GLU:HG2	1.93	0.68
1:C:103:ILE:HG13	1:C:233:TYR:CE2	2.28	0.67
1:A:13:ILE:HB	2:B:26:HIS:CD2	2.31	0.65
2:B:149:MET:HE3	2:B:153:ARG:HD3	1.78	0.65
1:E:224:ARG:NH2	4:E:401:NAG:O3	2.29	0.65
2:F:145:ASP:H	2:F:148:CYS:HB3	1.61	0.64
1:E:20:ASN:ND2	1:E:21:ASN:OD1	2.31	0.64
1:A:39:SER:HB3	1:A:315:ARG:HE	1.62	0.64
2:F:165:GLU:O	2:F:169:ASN:ND2	2.31	0.63
2:D:145:ASP:H	2:D:148:CYS:HB3	1.64	0.63
1:A:29:VAL:O	2:F:50:ASN:ND2	2.31	0.63
2:B:6:ILE:HG13	2:B:115:VAL:HG11	1.79	0.63
2:F:148:CYS:O	2:F:151:SER:HB3	1.99	0.62
1:A:310:ARG:NH1	2:B:90:ASP:OD1	2.30	0.62
1:E:17:TYR:CE2	2:F:6:ILE:HG13	2.34	0.62
1:C:28:THR:HG22	2:D:104:ASN:HB3	1.81	0.62
2:B:26:HIS:CG	2:B:149:MET:HG2	2.35	0.62
1:C:14:CYS:HA	2:D:137:CYS:HA	1.82	0.61
1:C:228:GLY:O	1:C:229:ARG:NH1	2.32	0.61
1:E:310:ARG:NH1	2:F:90:ASP:OD1	2.34	0.61
1:E:156:LYS:HD3	1:E:196:GLN:HB2	1.81	0.61
1:A:156:LYS:HD2	1:A:196:GLN:HB2	1.81	0.61
2:B:162:TYR:O	2:B:166:SER:OG	2.19	0.61
2:F:54:SER:O	2:F:58:LYS:NZ	2.30	0.60
1:E:21:ASN:OD1	1:E:21:ASN:N	2.35	0.60
1:E:14:CYS:O	2:F:25:HIS:N	2.34	0.60
2:B:146:ASP:O	2:B:150:GLU:N	2.31	0.60
1:E:277:CYS:SG	1:E:278:ASN:N	2.74	0.60
1:C:28:THR:O	1:C:32:LYS:NZ	2.34	0.60
1:C:212:ARG:HH11	1:E:216:GLU:HA	1.66	0.60
2:F:144:CYS:SG	2:F:145:ASP:N	2.75	0.58
2:D:144:CYS:SG	2:D:145:ASP:N	2.76	0.58
2:F:142:HIS:CD2	2:F:162:TYR:HB3	2.39	0.58
2:F:132:GLU:HG3	2:F:138:PHE:HE1	1.68	0.58
1:C:114:SER:HB3	1:C:262:ARG:NH1	2.19	0.58
1:C:216:GLU:O	1:C:220:ARG:NH2	2.37	0.57
2:B:60:ASN:ND2	2:B:61:THR:O	2.36	0.57
2:D:53:ASN:HB2	3:H:14:SER:HB3	1.84	0.57
2:F:141:TYR:HD1	2:F:166:SER:HB2	1.70	0.57
2:B:152:VAL:HG13	2:B:157:TYR:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:GLU:O	2:B:169:ASN:ND2	2.39	0.56
1:E:64:CYS:O	1:E:93:SER:HB3	2.06	0.56
1:E:48:ASN:O	1:E:50:LYS:HG3	2.05	0.56
1:A:22:SER:OG	1:A:36:VAL:O	2.23	0.56
2:F:145:ASP:OD1	2:F:162:TYR:OH	2.22	0.56
1:E:14:CYS:HB2	2:F:25:HIS:HB3	1.88	0.56
2:F:127:LYS:HE2	2:F:128:ASN:H	1.70	0.56
1:A:103:ILE:HG13	1:A:233:TYR:CE2	2.42	0.55
2:D:128:ASN:HB2	2:D:159:TYR:OH	2.07	0.55
2:F:158:ASP:HB3	2:F:161:LYS:HB2	1.88	0.55
2:B:71:ASN:OD1	2:B:74:GLU:HG3	2.07	0.55
1:C:131:GLU:OE2	1:C:133:THR:OG1	2.23	0.55
2:F:48:ILE:HD11	2:F:110:PHE:CD2	2.42	0.55
1:A:13:ILE:HG13	2:B:149:MET:CE	2.34	0.54
1:A:210:ASN:OD1	1:C:220:ARG:NE	2.33	0.54
1:E:320:LEU:HB3	2:F:111:HIS:CD2	2.42	0.54
1:A:323:ILE:HG21	2:B:12:GLY:HA2	1.89	0.54
2:D:117:ASN:ND2	2:F:4:GLY:HA3	2.21	0.54
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.43	0.54
1:E:124:PHE:HE1	1:E:254:PRO:HG2	1.72	0.54
2:F:70:PHE:CA	2:F:74:GLU:OE1	2.54	0.54
2:F:142:HIS:HD2	2:F:162:TYR:HB3	1.71	0.54
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.43	0.54
2:F:52:VAL:HG11	3:I:17:ILE:HD12	1.90	0.54
1:C:102:PHE:HB3	1:C:105:TYR:HB2	1.90	0.53
1:A:37:THR:HG23	1:A:320:LEU:O	2.07	0.53
2:B:50:ASN:HD21	1:C:32:LYS:HD3	1.73	0.53
1:E:215:PRO:HB3	1:E:250:ASN:ND2	2.23	0.53
2:F:132:GLU:HG3	2:F:138:PHE:CE1	2.44	0.53
2:D:127:LYS:NZ	2:F:132:GLU:O	2.42	0.53
2:B:5:ALA:HB1	2:B:115:VAL:HG22	1.90	0.53
2:D:170:ARG:CZ	2:D:170:ARG:HB2	2.39	0.53
2:F:49:THR:HG21	3:I:18:ALA:HB2	1.91	0.53
1:A:41:ASN:ND2	1:A:43:LEU:O	2.37	0.53
2:B:72:ASN:N	2:B:72:ASN:OD1	2.40	0.53
1:A:19:ALA:O	1:A:20:ASN:ND2	2.42	0.53
1:E:15:ILE:HD11	2:F:119:TYR:HB2	1.91	0.53
3:G:22:ALA:HB1	3:G:37:VAL:HA	1.91	0.53
1:A:265:SER:OG	1:A:266:GLY:N	2.41	0.52
2:B:150:GLU:HA	2:B:153:ARG:HE	1.73	0.52
2:B:142:HIS:CG	2:B:162:TYR:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:141:TYR:CD1	2:F:166:SER:HB2	2.45	0.52
1:C:210:ASN:HD21	1:E:220:ARG:NH2	2.07	0.52
2:D:128:ASN:O	2:D:170:ARG:NH2	2.42	0.52
1:C:15:ILE:HD11	2:D:119:TYR:HD1	1.75	0.52
2:F:3:PHE:CE2	2:F:113:SER:HB3	2.45	0.52
3:G:13:PHE:O	3:G:17:ILE:HG13	2.09	0.52
1:C:212:ARG:NH1	1:E:216:GLU:HA	2.25	0.52
1:E:164:LEU:O	1:E:246:GLU:HA	2.10	0.52
1:A:28:THR:HG22	2:B:104:ASN:HB3	1.91	0.52
2:F:159:TYR:N	2:F:160:PRO:HD2	2.26	0.51
1:C:73:ASN:HB3	1:C:76:CYS:SG	2.49	0.51
1:E:279:THR:OG1	1:E:280:LYS:N	2.43	0.51
2:D:3:PHE:CE2	2:D:113:SER:HB2	2.45	0.51
1:C:20:ASN:OD1	1:C:322:ASN:ND2	2.43	0.51
1:E:195:TYR:CE2	1:E:250:ASN:OD1	2.63	0.51
2:B:145:ASP:N	2:B:145:ASP:OD2	2.42	0.51
2:F:53:ASN:HB2	3:I:14:SER:HB2	1.93	0.51
2:B:142:HIS:ND1	2:B:143:LYS:O	2.44	0.51
1:A:174:LYS:HD2	1:A:259:ALA:HB1	1.93	0.51
1:E:220:ARG:HB2	1:E:227:ALA:O	2.11	0.50
1:C:210:ASN:HD21	1:E:220:ARG:HH21	1.59	0.50
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.46	0.50
2:B:72:ASN:ND2	1:E:208:LYS:HD2	2.26	0.50
2:D:119:TYR:HE1	2:D:136:GLY:HA2	1.76	0.50
2:D:119:TYR:CE1	2:D:136:GLY:HA2	2.47	0.50
2:F:5:ALA:HB2	2:F:116:ARG:HB2	1.92	0.50
2:D:167:LYS:HA	2:D:170:ARG:HB3	1.94	0.49
1:E:130:HIS:NE2	1:E:164:LEU:HB3	2.27	0.49
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.93	0.49
2:F:87:GLY:O	2:F:91:ILE:HD12	2.13	0.49
1:E:319:GLY:HA2	2:F:21:TRP:CZ2	2.48	0.49
1:E:305:CYS:O	2:F:62:GLN:N	2.45	0.48
1:E:114:SER:OG	1:E:262:ARG:NH1	2.45	0.48
2:B:98:LEU:HA	2:F:58:LYS:HE3	1.95	0.48
1:C:58:PRO:HB3	1:C:86:TYR:CZ	2.48	0.48
1:C:200:ALA:O	1:C:215:PRO:HD2	2.14	0.48
1:C:156:LYS:HD3	1:C:196:GLN:HB2	1.95	0.48
2:F:19:ASP:N	2:F:19:ASP:OD1	2.46	0.48
1:E:13:ILE:HD11	2:F:24:TYR:HB3	1.96	0.48
2:B:159:TYR:CG	2:B:160:PRO:HD3	2.48	0.48
1:A:152:LEU:HD23	1:A:154:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:HIS:HB2	2:B:165:GLU:HB3	1.95	0.48
2:B:55:VAL:HG22	2:B:56:ILE:HD13	1.95	0.48
2:D:109:ASP:OD1	2:D:110:PHE:N	2.47	0.47
1:A:18:HIS:ND1	2:B:20:GLY:O	2.44	0.47
1:E:32:LYS:HG3	1:E:33[A]:ASN:HB2	1.96	0.47
2:D:91:ILE:HD13	2:F:91:ILE:HG12	1.96	0.47
2:F:6:ILE:HD12	2:F:112:ASP:HA	1.97	0.47
1:C:37:THR:OG1	1:C:320:LEU:N	2.46	0.47
2:B:123:LYS:HB2	2:B:138:PHE:CZ	2.50	0.47
2:D:103:GLU:OE1	2:D:106:ARG:NH1	2.47	0.47
1:C:44:GLU:OE1	1:C:290:SER:OG	2.27	0.47
2:D:73:LEU:HD12	2:D:73:LEU:HA	1.72	0.47
2:B:167:LYS:HD3	2:D:173:ILE:HG13	1.97	0.47
3:I:52:HIS:O	3:I:54:GLU:N	2.48	0.47
1:E:15:ILE:HG22	2:F:24:TYR:CD1	2.50	0.47
1:E:110:GLU:OE2	2:F:68:LYS:NZ	2.48	0.47
2:D:91:ILE:CD1	2:F:91:ILE:HG12	2.45	0.47
2:F:38:GLN:O	2:F:42:GLN:NE2	2.44	0.47
2:D:91:ILE:HD12	2:D:91:ILE:C	2.35	0.46
2:D:54:SER:O	2:D:58:LYS:HG2	2.15	0.46
1:A:127:TRP:HZ3	1:A:164:LEU:HD13	1.80	0.46
1:E:32:LYS:HG3	1:E:33[B]:ASN:HB2	1.97	0.46
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.97	0.46
1:E:71:LEU:HD22	1:E:151:LEU:HD11	1.98	0.46
2:B:117:ASN:ND2	2:D:1:GLY:O	2.45	0.45
2:B:152:VAL:HG13	2:B:157:TYR:CE2	2.50	0.45
1:C:122:GLU:OE1	1:C:125:PRO:HA	2.16	0.45
2:F:122:VAL:HA	2:F:125:GLN:HB2	1.98	0.45
1:C:100:GLY:HA3	1:C:230:MET:O	2.16	0.45
1:C:174:LYS:HZ1	1:C:261:ASN:HD21	1.64	0.45
1:E:223:VAL:HG12	1:E:224:ARG:HG3	1.98	0.45
1:A:126:SER:HB2	1:A:127:TRP:CD1	2.52	0.45
1:A:48:ASN:O	1:A:50:LYS:HG2	2.17	0.45
2:D:70:PHE:C	2:D:74:GLU:OE1	2.55	0.45
1:A:36:VAL:HA	1:A:321:ARG:HA	1.98	0.45
2:F:121:LYS:HG3	2:F:122:VAL:N	2.32	0.45
1:A:43:LEU:HB2	1:A:314:LEU:HB2	1.99	0.45
2:F:55:VAL:HA	2:F:58:LYS:NZ	2.32	0.44
1:A:293:PRO:HB3	2:B:56:ILE:HD12	1.99	0.44
1:E:122:GLU:HG3	1:E:256:TYR:CZ	2.52	0.44
2:B:48:ILE:O	2:B:52:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:SER:O	1:E:196:GLN:NE2	2.46	0.44
1:E:26:VAL:HG13	1:E:36:VAL:HG21	1.99	0.44
1:C:73:ASN:ND2	1:C:95(A):GLY:O	2.41	0.44
1:A:186:PRO:HB3	1:A:227:ALA:HB3	2.00	0.44
2:D:148:CYS:O	2:D:151:SER:HB3	2.18	0.44
1:E:127:TRP:CZ3	1:E:164:LEU:HD13	2.53	0.44
2:D:142:HIS:HD2	2:D:143:LYS:O	2.01	0.44
2:B:3:PHE:CZ	2:D:2:LEU:HG	2.53	0.44
2:F:42:GLN:HG3	3:I:40:TYR:HA	1.99	0.44
1:E:73:ASN:HB3	1:E:76:CYS:SG	2.57	0.44
1:A:73:ASN:HB3	1:A:76:CYS:SG	2.58	0.44
1:E:15:ILE:HG22	2:F:24:TYR:HD1	1.83	0.43
2:B:88:PHE:CE1	2:D:87:GLY:HA3	2.54	0.43
1:E:320:LEU:HD23	1:E:320:LEU:H	1.83	0.43
1:E:314:LEU:HD12	1:E:314:LEU:HA	1.76	0.43
1:C:147:PHE:CG	1:C:148:TYR:N	2.85	0.43
2:B:150:GLU:HB2	2:B:153:ARG:HH21	1.83	0.43
2:D:146:ASP:OD1	2:D:146:ASP:N	2.51	0.43
1:A:318:THR:HA	2:B:48:ILE:HD11	2.01	0.43
1:A:323:ILE:H	1:A:323:ILE:HG13	1.49	0.43
1:A:130:HIS:CE1	1:A:164:LEU:HB3	2.54	0.43
1:E:190:ASP:O	1:E:194:LEU:HG	2.19	0.43
2:B:52:VAL:HG11	3:G:17:ILE:CD1	2.48	0.43
2:B:111:HIS:O	2:B:115:VAL:HG12	2.18	0.43
2:B:87:GLY:HA3	2:F:88:PHE:CZ	2.54	0.43
1:A:54(A):LYS:N	1:A:54(A):LYS:HD2	2.34	0.43
1:C:314:LEU:HD22	2:D:100:VAL:HG21	2.00	0.43
2:D:151:SER:O	2:D:154:ASN:ND2	2.53	0.42
1:E:228:GLY:O	1:E:229:ARG:NH1	2.48	0.42
1:C:284:PRO:HG2	1:C:298:HIS:CE1	2.54	0.42
2:B:130:ALA:HB2	2:B:140:PHE:HD1	1.84	0.42
1:A:316:MET:HE1	2:B:52:VAL:HA	2.01	0.42
1:E:26:VAL:HG12	1:E:315:ARG:HG2	2.02	0.42
2:B:50:ASN:HD21	1:C:32:LYS:CD	2.33	0.42
2:D:51:LYS:HE3	2:D:103:GLU:HB3	2.00	0.42
2:F:20:GLY:HA2	3:I:25:PHE:CZ	2.55	0.42
2:F:53:ASN:HB2	3:I:14:SER:CB	2.49	0.42
1:A:63:LYS:O	1:A:95:ASN:HB2	2.20	0.42
1:C:71:LEU:HD22	1:C:151:LEU:HD11	2.02	0.42
1:E:37:THR:HG23	1:E:320:LEU:O	2.19	0.42
1:E:127:TRP:HZ3	1:E:164:LEU:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LEU:HD23	1:E:279:THR:O	2.19	0.42
1:C:134:GLY:CA	1:C:153:TRP:HB3	2.49	0.42
1:E:103:ILE:HG13	1:E:233:TYR:CE2	2.54	0.42
1:C:215:PRO:HB3	1:C:250:ASN:ND2	2.35	0.42
1:C:98:TYR:CD2	1:C:230:MET:HB2	2.55	0.42
2:F:103:GLU:O	2:F:107:THR:HG23	2.19	0.42
1:E:211:ARG:NH1	5:E:506:HOH:O	2.48	0.42
2:B:3:PHE:CZ	2:B:113:SER:HB2	2.55	0.41
2:F:76:ARG:HB2	5:F:202:HOH:O	2.20	0.41
2:D:81:ASN:OD1	2:F:80:LEU:HD13	2.20	0.41
2:F:60:ASN:N	2:F:60:ASN:OD1	2.51	0.41
1:A:318:THR:O	2:B:48:ILE:HD13	2.20	0.41
1:E:71:LEU:O	1:E:148:TYR:HB3	2.19	0.41
1:A:295:GLN:HG2	1:A:306:PRO:HB2	2.03	0.41
2:B:20:GLY:HA2	3:G:25:PHE:CZ	2.56	0.41
1:E:95(A):GLY:HA3	5:E:509:HOH:O	2.19	0.41
1:E:102:PHE:HB3	1:E:105:TYR:HB2	2.03	0.41
2:B:26:HIS:HE1	2:B:28:ASN:CG	2.23	0.41
1:A:20:ASN:CA	1:A:322:ASN:HD21	2.34	0.41
2:F:129:ASN:OD1	2:F:159:TYR:OH	2.36	0.41
1:E:54:LEU:HB2	1:E:85:SER:OG	2.20	0.41
1:E:295:GLN:HG2	1:E:306:PRO:HB2	2.03	0.41
2:D:47:GLY:HA2	1:E:30:LEU:O	2.21	0.41
1:E:73:ASN:HA	1:E:74:PRO:HD3	1.83	0.41
1:C:174:LYS:HZ3	1:C:261:ASN:HD21	1.66	0.41
2:B:98:LEU:CA	2:F:58:LYS:HE3	2.50	0.41
1:E:215:PRO:HG3	1:E:250:ASN:ND2	2.36	0.41
1:A:85[B]:SER:HG	1:A:86:TYR:HD2	1.67	0.41
1:A:204:VAL:HG22	1:A:245:PHE:CD1	2.55	0.41
1:A:191:GLN:NE2	1:A:195:TYR:HD2	2.19	0.41
1:C:274:VAL:HG23	5:C:511:HOH:O	2.21	0.41
1:C:58:PRO:HB3	1:C:86:TYR:CE1	2.56	0.40
2:D:58:LYS:HA	2:D:58:LYS:HD3	1.74	0.40
2:B:140:PHE:HD2	2:B:144:CYS:HB2	1.87	0.40
2:F:28:ASN:ND2	2:F:146:ASP:OD1	2.48	0.40
1:A:242:THR:HB	1:C:221:PRO:HB3	2.03	0.40
2:F:6:ILE:HD11	2:F:115:VAL:HG21	2.04	0.40
1:C:220:ARG:HD3	1:C:229:ARG:HG2	2.03	0.40
1:E:69:TRP:HZ3	1:E:87:ILE:HD13	1.85	0.40
1:C:12:THR:HA	2:D:138:PHE:O	2.20	0.40
2:D:53:ASN:O	2:D:57:GLU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:32:ASP:O	3:I:36:LYS:N	2.51	0.40
2:B:58:LYS:HB3	2:D:94:TYR:HD1	1.85	0.40
1:C:24:ASP:N	1:C:24:ASP:OD1	2.54	0.40
2:B:99:LEU:HD13	2:D:98:LEU:HD21	2.03	0.40
1:C:59:LEU:HB2	1:C:84:TRP:HB3	2.04	0.40
2:B:6:ILE:CG1	2:B:115:VAL:HG11	2.50	0.40
1:E:105:TYR:CE2	1:E:109:ARG:HD2	2.56	0.40
2:F:26:HIS:ND1	2:F:26:HIS:O	2.54	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	325/331 (98%)	316 (97%)	9 (3%)	0	100 100
1	C	322/331 (97%)	314 (98%)	8 (2%)	0	100 100
1	E	322/331 (97%)	309 (96%)	13 (4%)	0	100 100
2	B	171/179 (96%)	160 (94%)	11 (6%)	0	100 100
2	D	172/179 (96%)	162 (94%)	10 (6%)	0	100 100
2	F	170/179 (95%)	157 (92%)	13 (8%)	0	100 100
3	G	43/74 (58%)	39 (91%)	4 (9%)	0	100 100
3	H	45/74 (61%)	41 (91%)	3 (7%)	1 (2%)	8 22
3	I	45/74 (61%)	40 (89%)	5 (11%)	0	100 100
All	All	1615/1752 (92%)	1538 (95%)	76 (5%)	1 (0%)	56 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	26	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	282/285 (99%)	251 (89%)	31 (11%)	8 18
1	C	279/285 (98%)	256 (92%)	23 (8%)	14 32
1	E	279/285 (98%)	246 (88%)	33 (12%)	6 15
2	B	148/152 (97%)	127 (86%)	21 (14%)	4 10
2	D	149/152 (98%)	127 (85%)	22 (15%)	4 9
2	F	147/152 (97%)	122 (83%)	25 (17%)	2 6
3	G	18/66 (27%)	13 (72%)	5 (28%)	0 1
3	H	17/66 (26%)	15 (88%)	2 (12%)	6 15
3	I	15/66 (23%)	14 (93%)	1 (7%)	20 44
All	All	1334/1509 (88%)	1171 (88%)	163 (12%)	6 14

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	15	ILE
1	A	21	ASN
1	A	22	SER
1	A	25	THR
1	A	29	VAL
1	A	32	LYS
1	A	36	VAL
1	A	40	VAL
1	A	46	SER
1	A	95	ASN
1	A	102	PHE
1	A	112	LEU
1	A	118	PHE

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Mol	Chain	Res	Type
1	A	133(A)	LYS
1	A	155	THR
1	A	179	LEU
1	A	193	SER
1	A	194	LEU
1	A	199	ASP
1	A	214	THR
1	A	268	ILE
1	A	291	SER
1	A	309	VAL
1	A	313	LYS
1	A	314	LEU
1	A	315	ARG
1	A	318	THR
1	A	321	ARG
1	A	323	ILE
1	A	326	ILE
2	B	18	ILE
2	B	22	TYR
2	B	38	GLN
2	B	42	GLN
2	B	55	VAL
2	B	61	THR
2	B	115	VAL
2	B	121	LYS
2	B	132	GLU
2	B	135	ASN
2	B	144	CYS
2	B	145	ASP
2	B	151	SER
2	B	152	VAL
2	B	157	TYR
2	B	159	TYR
2	B	161	LYS
2	B	165	GLU
2	B	166	SER
2	B	168	LEU
2	B	171	GLU
1	C	12	THR
1	C	13	ILE
1	C	14	CYS
1	C	22	SER

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Mol	Chain	Res	Type
1	C	24	ASP
1	C	29	VAL
1	C	36	VAL
1	C	45	ASP
1	C	83	SER
1	C	94	GLU
1	C	102	PHE
1	C	118	PHE
1	C	125(C)	SER
1	C	133	THR
1	C	136	THR
1	C	155	THR
1	C	165	SER
1	C	211	ARG
1	C	277	CYS
1	C	290	SER
1	C	304	GLU
1	C	307	LYS
1	C	312	THR
2	D	2	LEU
2	D	10	ILE
2	D	15	THR
2	D	22	TYR
2	D	29	GLU
2	D	30	GLN
2	D	42	GLN
2	D	61	THR
2	D	63	PHE
2	D	68	LYS
2	D	73	LEU
2	D	106	ARG
2	D	109	ASP
2	D	112	ASP
2	D	119	TYR
2	D	132	GLU
2	D	140	PHE
2	D	144	CYS
2	D	152	VAL
2	D	154	ASN
2	D	163	SER
2	D	164	GLU
1	E	20	ASN

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Mol	Chain	Res	Type
1	E	21	ASN
1	E	22	SER
1	E	23	THR
1	E	25	THR
1	E	28	THR
1	E	32	LYS
1	E	35	THR
1	E	36	VAL
1	E	46	SER
1	E	63	LYS
1	E	81	THR
1	E	93	SER
1	E	94	GLU
1	E	118	PHE
1	E	125(B)	THR
1	E	159	SER
1	E	171	ASN
1	E	189	THR
1	E	192	GLN
1	E	193	SER
1	E	208	LYS
1	E	214	THR
1	E	238	GLU
1	E	275	HIS
1	E	277	CYS
1	E	278	ASN
1	E	279	THR
1	E	280	LYS
1	E	312	THR
1	E	313	LYS
1	E	314	LEU
1	E	318	THR
2	F	10	ILE
2	F	15	THR
2	F	19	ASP
2	F	49	THR
2	F	56	ILE
2	F	61	THR
2	F	68	LYS
2	F	75	ARG
2	F	122	VAL
2	F	126	LEU

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Mol	Chain	Res	Type
2	F	127	LYS
2	F	128	ASN
2	F	131	LYS
2	F	133	ILE
2	F	138	PHE
2	F	139	GLU
2	F	140	PHE
2	F	143	LYS
2	F	152	VAL
2	F	156	THR
2	F	161	LYS
2	F	164	GLU
2	F	166	SER
2	F	170	ARG
2	F	171	GLU
3	G	11	TRP
3	G	14	SER
3	G	21	ILE
3	G	24	SER
3	G	54	GLU
3	H	14	SER
3	H	19	PHE
3	I	24	SER

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	20	ASN
2	B	26	HIS
2	B	50	ASN
2	B	60	ASN
2	B	79	ASN
2	B	169	ASN
1	C	210	ASN
1	C	261	ASN
1	C	275	HIS
2	D	117	ASN
2	D	142	HIS
1	E	20	ASN
1	E	250	ASN
2	F	111	HIS
2	F	154	ASN

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

9 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	$\#\|Z\| > 2$
4	NAG	A	401	1,4	14,14,15	0.47	0	15,19,21	2.36	4 (26%)
4	NAG	A	402	4	14,14,15	0.59	0	15,19,21	1.79	3 (20%)
4	BMA	A	403	4	11,11,12	0.58	0	14,15,17	0.93	0
4	NAG	C	401	1,4	14,14,15	0.68	0	15,19,21	2.30	4 (26%)
4	NAG	C	402	4	14,14,15	0.73	1 (7%)	15,19,21	1.54	2 (13%)
4	BMA	C	403	4	11,11,12	0.66	0	14,15,17	0.99	0
4	NAG	E	401	1,4	14,14,15	0.47	0	15,19,21	1.72	4 (26%)
4	NAG	E	402	4	14,14,15	0.70	0	15,19,21	1.41	2 (13%)
4	BMA	E	403	4	11,11,12	0.58	0	14,15,17	0.68	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	NAG	A	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	402	4	-	0/6/23/26	0/1/1/1
4	BMA	A	403	4	-	0/2/19/22	0/1/1/1
4	NAG	C	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	402	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	C	403	4	-	0/2/19/22	0/1/1/1
4	NAG	E	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	402	4	-	0/6/23/26	0/1/1/1
4	BMA	E	403	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	NAG	O5-C1	-2.11	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	402	NAG	C2-N2-C7	-4.22	117.61	123.04
4	C	402	NAG	C2-N2-C7	-2.80	119.44	123.04
4	A	401	NAG	C2-N2-C7	-2.59	119.71	123.04
4	C	401	NAG	C6-C5-C4	-2.58	106.65	113.02
4	C	401	NAG	O7-C7-C8	-2.55	117.37	122.06
4	E	401	NAG	C6-C5-C4	-2.48	106.89	113.02
4	A	401	NAG	C6-C5-C4	-2.41	107.08	113.02
4	A	401	NAG	O4-C4-C5	-2.28	103.19	109.24
4	E	401	NAG	C3-C2-N2	-2.27	105.13	110.56
4	A	402	NAG	O4-C4-C3	-2.12	105.56	110.34
4	C	401	NAG	C8-C7-N2	2.09	120.11	116.11
4	A	402	NAG	C3-C4-C5	2.19	114.01	110.20
4	E	402	NAG	C3-C4-C5	2.25	114.12	110.20
4	E	401	NAG	C1-O5-C5	2.62	115.58	112.25
4	C	402	NAG	C1-O5-C5	3.62	116.85	112.25
4	E	401	NAG	O5-C5-C6	4.39	116.86	107.35
4	A	402	NAG	C1-O5-C5	4.97	118.55	112.25
4	C	401	NAG	C1-O5-C5	7.19	121.37	112.25
4	A	401	NAG	C1-O5-C5	7.46	121.72	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	NAG	1	0

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	325/331 (98%)	-0.07	11 (3%) 49 49	25, 53, 103, 161	0
1	C	323/331 (97%)	-0.16	4 (1%) 81 81	30, 58, 97, 120	0
1	E	323/331 (97%)	-0.01	5 (1%) 76 76	34, 62, 106, 155	0
2	B	173/179 (96%)	1.22	40 (23%) 1 1	36, 105, 151, 174	0
2	D	173/179 (96%)	0.90	29 (16%) 2 2	28, 102, 129, 153	0
2	F	171/179 (95%)	1.45	46 (26%) 1 1	28, 121, 172, 183	0
3	G	45/74 (60%)	1.31	11 (24%) 1 1	63, 121, 145, 159	0
3	H	47/74 (63%)	1.47	15 (31%) 1 0	100, 125, 158, 186	0
3	I	47/74 (63%)	2.79	29 (61%) 0 0	111, 156, 179, 208	0
All	All	1627/1752 (92%)	0.49	190 (11%) 6 5	25, 74, 153, 208	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	27	ASN	12.0
3	I	8	GLY	11.6
2	B	138	PHE	7.7
3	I	43	GLY	7.5
2	F	149	MET	7.4
2	F	141	TYR	6.9
2	F	1	GLY	6.5
2	F	160	PRO	6.4
3	G	18	ALA	6.3
1	A	15	ILE	6.2
3	I	53	TYR	5.9
3	I	31	PRO	5.8
2	B	33	GLY	5.8
3	I	45	THR	5.7
2	B	128	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
3	I	11	TRP	5.4
2	B	148	CYS	5.4
3	H	23	LEU	5.3
1	A	11	ASP	5.3
2	D	126	LEU	5.3
3	I	48	GLU	5.2
2	B	140	PHE	5.1
2	D	31	GLY	5.1
2	D	173	ILE	5.1
2	D	168	LEU	5.1
3	H	28	LYS	5.1
2	B	26	HIS	5.0
3	G	23	LEU	5.0
2	B	25	HIS	5.0
2	F	22	TYR	4.9
2	D	62	GLN	4.8
2	B	24	TYR	4.7
2	D	141	TYR	4.7
3	I	49	VAL	4.6
1	A	12	THR	4.6
2	B	160	PRO	4.6
3	G	19	PHE	4.5
2	F	140	PHE	4.5
1	A	13	ILE	4.5
2	D	18	ILE	4.4
2	F	158	ASP	4.4
2	F	142	HIS	4.4
3	I	32	ASP	4.4
2	F	107	THR	4.4
2	B	167	LYS	4.3
2	B	159	TYR	4.1
2	F	33	GLY	4.1
3	I	44	ARG	4.1
2	F	131	LYS	4.1
3	I	10	PRO	4.0
2	B	30	GLN	4.0
3	I	9	ARG	4.0
2	B	35	ALA	3.9
2	F	34	TYR	3.9
3	I	40	TYR	3.9
3	G	38	ALA	3.9
2	F	32	SER	3.8

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Mol	Chain	Res	Type	RSRZ
3	G	47	GLU	3.8
2	F	41	THR	3.7
2	B	1	GLY	3.7
2	B	146	ASP	3.7
3	H	29	ASP	3.7
1	E	16	GLY	3.7
1	A	34	VAL	3.7
2	F	148	CYS	3.6
3	H	24	SER	3.6
2	F	161	LYS	3.6
1	A	326	ILE	3.5
3	G	28	LYS	3.5
2	F	157	TYR	3.5
3	G	17	ILE	3.4
3	I	47	GLU	3.4
2	F	139	GLU	3.4
2	B	145	ASP	3.3
3	G	45	THR	3.3
2	B	29	GLU	3.3
2	D	16	GLY	3.3
3	H	11	TRP	3.3
2	F	170	ARG	3.3
2	F	164	GLU	3.3
3	I	29	ASP	3.3
3	H	34	TRP	3.2
2	B	126	LEU	3.2
2	B	157	TYR	3.2
3	H	8	GLY	3.1
2	F	128	ASN	3.1
3	I	30	THR	3.1
2	B	36	ALA	3.1
2	D	106	ARG	3.1
2	F	135	ASN	3.1
3	H	40	TYR	3.1
2	D	35	ALA	3.0
1	A	323	ILE	3.0
2	B	158	ASP	3.0
2	F	114	ASN	3.0
3	I	36	LYS	3.0
2	F	19	ASP	2.9
1	A	16	GLY	2.9
2	B	62	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
3	I	19	PHE	2.9
2	F	153	ARG	2.9
2	B	139	GLU	2.9
2	D	64	THR	2.9
2	F	23	GLY	2.9
1	C	14	CYS	2.9
2	B	155	GLY	2.9
2	B	162	TYR	2.9
3	I	46	PRO	2.9
3	I	33	ARG	2.8
1	A	324	PRO	2.8
2	B	127	LYS	2.8
2	D	19	ASP	2.8
2	B	124	SER	2.8
2	B	163	SER	2.8
2	D	143	LYS	2.8
2	D	170	ARG	2.8
2	F	61	THR	2.8
2	F	155	GLY	2.8
2	B	168	LEU	2.8
2	D	133	ILE	2.8
2	B	23	GLY	2.7
2	D	28	ASN	2.7
3	H	9	ARG	2.7
1	E	15	ILE	2.7
2	D	66	VAL	2.7
2	D	172	GLU	2.7
2	B	2	LEU	2.6
2	F	9	PHE	2.6
3	I	37	VAL	2.6
3	I	54	GLU	2.6
3	G	48	GLU	2.6
3	H	26	THR	2.6
3	I	52	HIS	2.6
1	E	12	THR	2.5
2	D	61	THR	2.5
3	H	32	ASP	2.5
2	F	4	GLY	2.5
2	F	31	GLY	2.5
2	F	125	GLN	2.5
2	F	37	ASP	2.5
3	H	47	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	320	LEU	2.5
2	B	3	PHE	2.5
2	D	138	PHE	2.4
3	I	41	VAL	2.4
3	H	44	ARG	2.4
2	B	170	ARG	2.4
2	D	65	ALA	2.4
3	I	50	LYS	2.4
2	F	124	SER	2.4
2	F	21	TRP	2.4
2	B	164	GLU	2.4
2	B	144	CYS	2.4
2	D	136	GLY	2.3
3	I	27	ASN	2.3
2	F	59	MET	2.3
3	I	34	TRP	2.3
2	B	106	ARG	2.3
2	D	13	GLY	2.3
1	A	322	ASN	2.3
2	F	162	TYR	2.3
1	C	324	PRO	2.2
2	D	38	GLN	2.2
2	F	24	TYR	2.2
2	F	143	LYS	2.2
2	F	26	HIS	2.2
3	G	37	VAL	2.2
1	C	16	GLY	2.2
2	B	12	GLY	2.2
3	G	25	PHE	2.2
3	I	18	ALA	2.2
2	F	106	ARG	2.1
2	B	39	LYS	2.1
2	B	61	THR	2.1
2	F	48	ILE	2.1
1	C	13	ILE	2.1
3	I	38	ALA	2.1
2	D	23	GLY	2.1
2	D	115	VAL	2.1
2	B	13	GLY	2.1
2	D	118	LEU	2.1
2	D	29	GLU	2.1
2	F	18	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	112	ASP	2.0
1	E	280	LYS	2.0
2	D	162	TYR	2.0
3	H	19	PHE	2.0
1	E	317	ALA	2.0
2	F	102	LEU	2.0
2	F	144	CYS	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^{th} 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^2)	Q<0.9
4	NAG	A	401	14/15	0.93	0.17	-0.14	48,60,67,72	0
4	NAG	E	401	14/15	0.95	0.16	-0.24	38,50,64,74	0
4	NAG	C	401	14/15	0.96	0.12	-1.18	27,47,62,74	0
4	NAG	C	402	14/15	0.95	0.14	-	67,76,88,95	0
4	BMA	E	403	11/12	0.84	0.18	-	97,99,109,109	0
4	BMA	C	403	11/12	0.67	0.24	-	98,102,104,105	0
4	NAG	E	402	14/15	0.89	0.15	-	72,78,85,92	0
4	BMA	A	403	11/12	0.78	0.21	-	89,94,107,110	0
4	NAG	A	402	14/15	0.92	0.13	-	51,65,82,82	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.