Full wwPDB X-ray Structure Validation Report (i)

May 9, 2023 – 01:51 pm BST

PDB ID	:	7ZQT
Title	:	Helicobacter pylori adhesin BabA bound to neutralising human antibody.
Authors	:	Moonens, K.; Boren, T.
Deposited on	:	2022-05-03
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

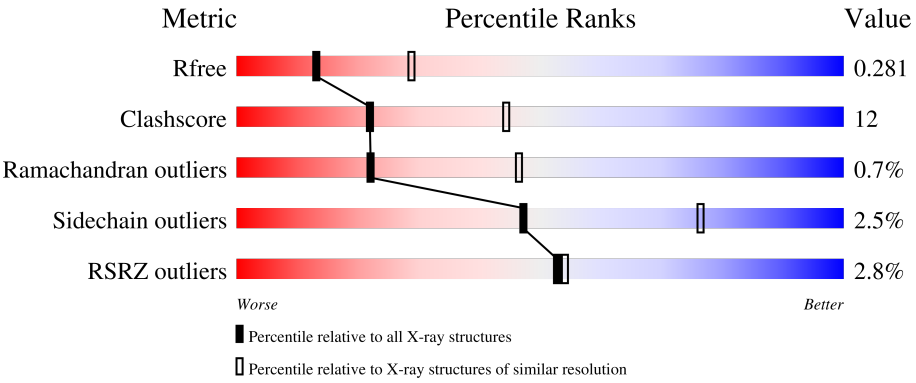
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	466	68% 18% · 14%
1	E	466	72% 16% · 11%
2	B	120	11% 57% 34% · 8%
2	F	120	4% 66% 26% · 8%
3	C	222	4% 58% 23% 5% 15%

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Mol	Chain	Length	Quality of chain
3	G	222	
4	D	211	
4	H	211	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13999 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 Adhesin binding fucosylated histo-blood group antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			2983	1840	513	617	13			
1	E	413	Total	C	N	O	S	0	0	0
			3077	1900	528	636	13			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	expression tag	UNP O52269
A	4	SER	-	expression tag	UNP O52269
A	5	TRP	-	expression tag	UNP O52269
A	6	SER	-	expression tag	UNP O52269
A	7	HIS	-	expression tag	UNP O52269
A	8	PRO	-	expression tag	UNP O52269
A	9	GLN	-	expression tag	UNP O52269
A	10	PHE	-	expression tag	UNP O52269
A	11	GLU	-	expression tag	UNP O52269
A	12	LYS	-	expression tag	UNP O52269
A	13	SER	-	expression tag	UNP O52269
A	14	GLY	-	expression tag	UNP O52269
A	15	GLY	-	expression tag	UNP O52269
A	16	GLY	-	expression tag	UNP O52269
A	17	GLY	-	expression tag	UNP O52269
A	18	GLY	-	expression tag	UNP O52269
A	19	LEU	-	expression tag	UNP O52269
A	20	VAL	-	expression tag	UNP O52269
A	21	PRO	-	expression tag	UNP O52269
A	22	ARG	-	expression tag	UNP O52269
A	23	GLY	-	expression tag	UNP O52269
A	24	SER	-	expression tag	UNP O52269
A	461	GLY	-	expression tag	UNP O52269
A	462	SER	-	expression tag	UNP O52269
A	463	HIS	-	expression tag	UNP O52269

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Chain	Residue	Modelled	Actual	Comment	Reference
A	464	HIS	-	expression tag	UNP O52269
A	465	HIS	-	expression tag	UNP O52269
A	466	HIS	-	expression tag	UNP O52269
A	467	HIS	-	expression tag	UNP O52269
A	468	HIS	-	expression tag	UNP O52269
E	3	ALA	-	expression tag	UNP O52269
E	4	SER	-	expression tag	UNP O52269
E	5	TRP	-	expression tag	UNP O52269
E	6	SER	-	expression tag	UNP O52269
E	7	HIS	-	expression tag	UNP O52269
E	8	PRO	-	expression tag	UNP O52269
E	9	GLN	-	expression tag	UNP O52269
E	10	PHE	-	expression tag	UNP O52269
E	11	GLU	-	expression tag	UNP O52269
E	12	LYS	-	expression tag	UNP O52269
E	13	SER	-	expression tag	UNP O52269
E	14	GLY	-	expression tag	UNP O52269
E	15	GLY	-	expression tag	UNP O52269
E	16	GLY	-	expression tag	UNP O52269
E	17	GLY	-	expression tag	UNP O52269
E	18	GLY	-	expression tag	UNP O52269
E	19	LEU	-	expression tag	UNP O52269
E	20	VAL	-	expression tag	UNP O52269
E	21	PRO	-	expression tag	UNP O52269
E	22	ARG	-	expression tag	UNP O52269
E	23	GLY	-	expression tag	UNP O52269
E	24	SER	-	expression tag	UNP O52269
E	461	GLY	-	expression tag	UNP O52269
E	462	SER	-	expression tag	UNP O52269
E	463	HIS	-	expression tag	UNP O52269
E	464	HIS	-	expression tag	UNP O52269
E	465	HIS	-	expression tag	UNP O52269
E	466	HIS	-	expression tag	UNP O52269
E	467	HIS	-	expression tag	UNP O52269
E	468	HIS	-	expression tag	UNP O52269

- Molecule 2 is a protein called Nanobody Nb19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	110	Total	C	N	O	S	0	0	0
			844	529	152	158	5			
2	F	111	Total	C	N	O	S	0	0	0
			851	534	153	159	5			

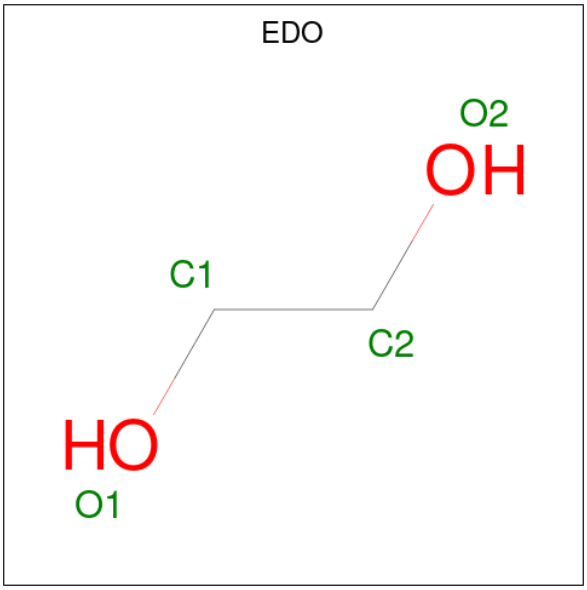
- Molecule 3 is a protein called VH domain human IgG antibody ABbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	189	Total	C	N	O	S	0	0	0
			1392	877	236	274	5			
3	G	213	Total	C	N	O	S	0	0	0
			1580	994	270	310	6			

- Molecule 4 is a protein called VL domain human IgG antibody ABbA.

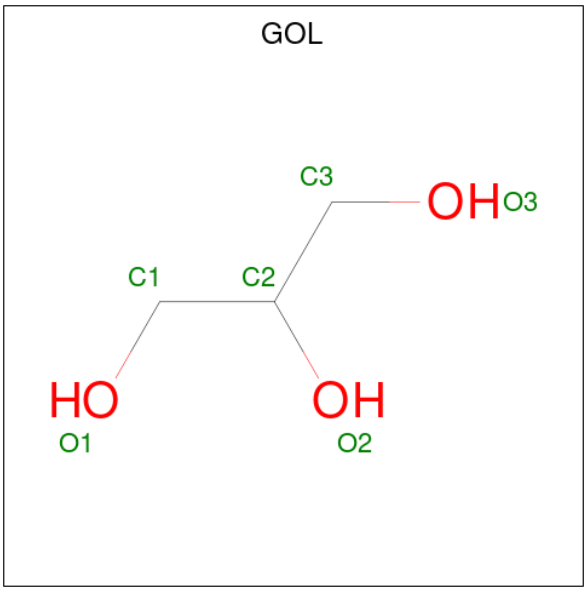
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	211	Total	C	N	O	S	0	0	0
			1624	1017	271	331	5			
4	H	211	Total	C	N	O	S	0	0	0
			1624	1017	271	331	5			

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

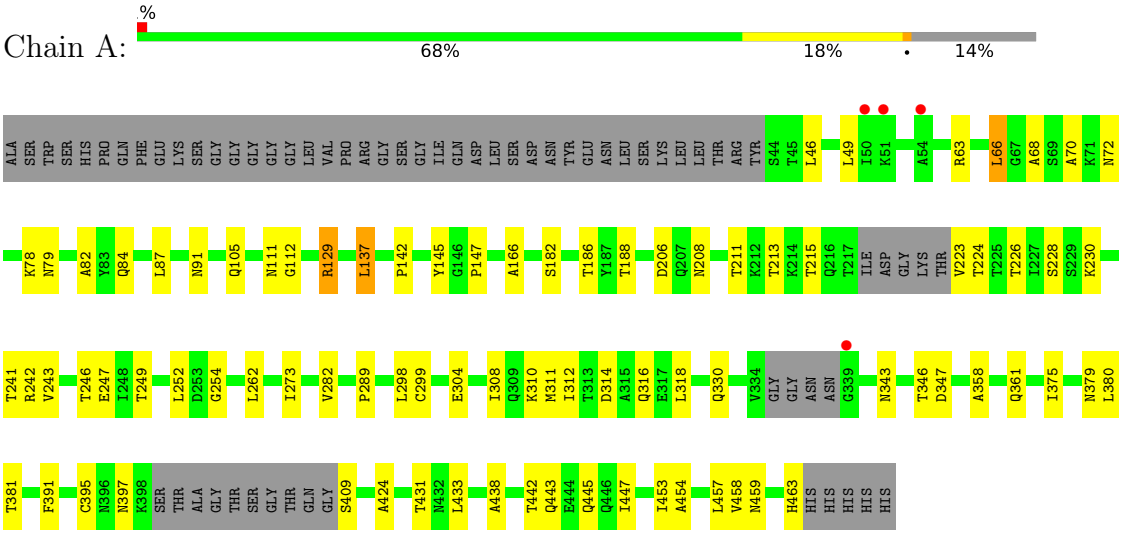
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	E	1	Total O 1 1	0	0
7	H	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

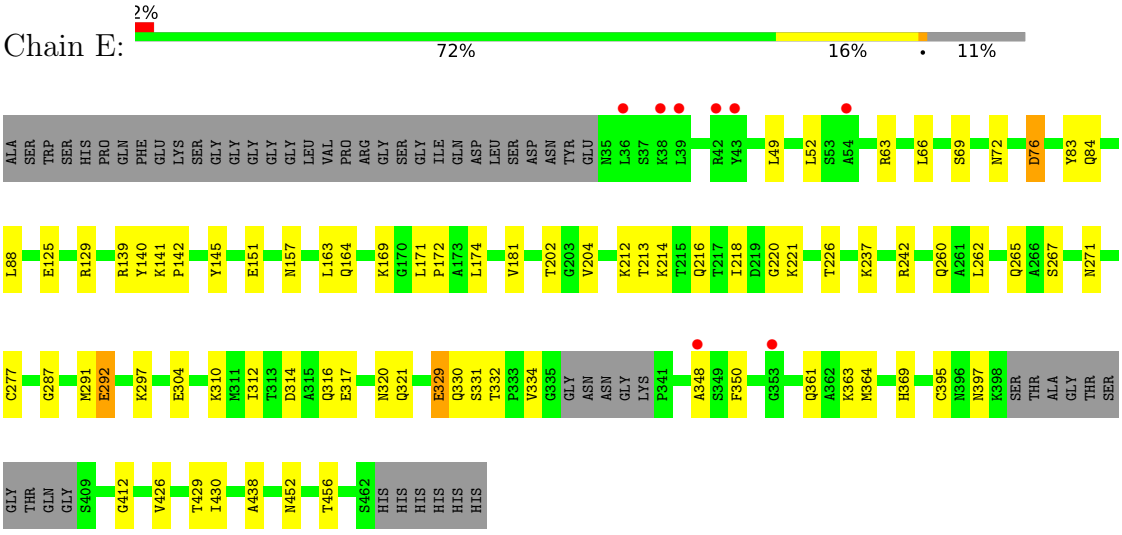
• Molecule 1: Adhesin binding fucosylated histo-blood group antigen

Chain A:



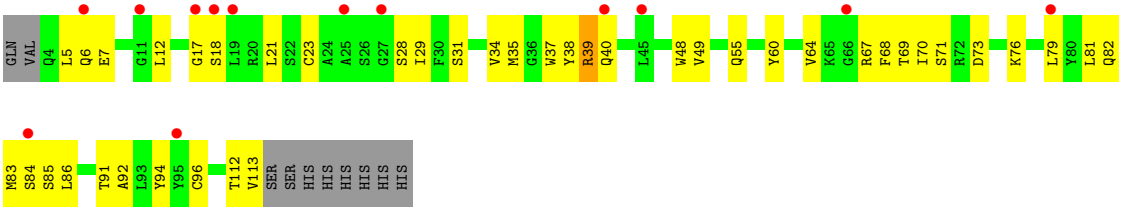
• Molecule 1: Adhesin binding fucosylated histo-blood group antigen

Chain E:



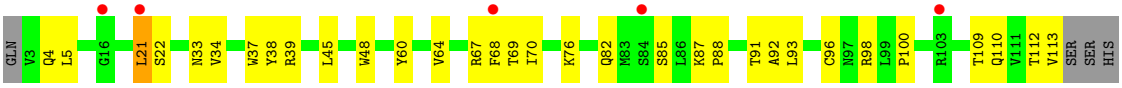
• Molecule 2: Nanobody Nb19

Chain B:



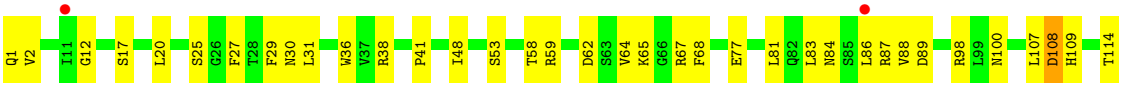
• Molecule 2: Nanobody Nb19

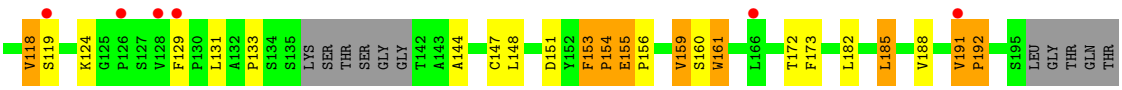
Chain F:



• Molecule 3: VH domain human IgG antibody ABbA

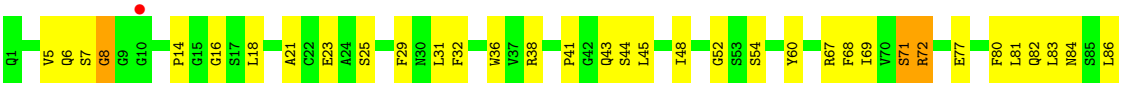
Chain C:

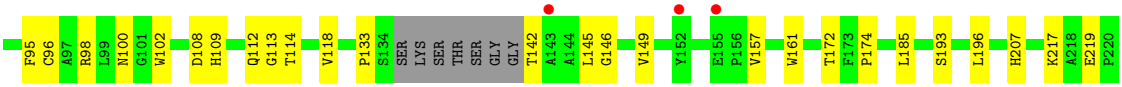




• Molecule 3: VH domain human IgG antibody ABbA

Chain G:



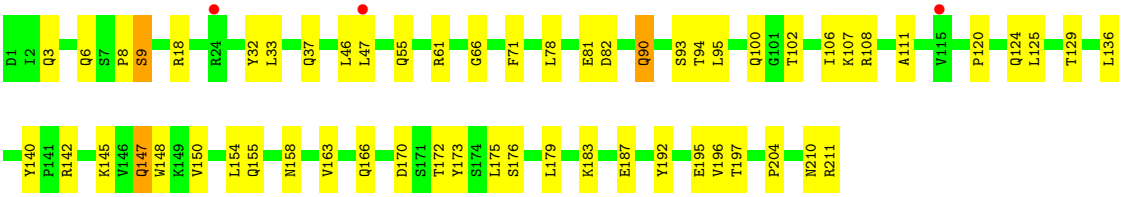


• Molecule 4: VL domain human IgG antibody ABbA

Chain D:

• Molecule 4: VL domain human IgG antibody ABbA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.70Å 68.40Å 176.60Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	48.28 – 2.70 48.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.28-2.70) 99.1 (48.28-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.225 , 0.281 0.225 , 0.281	Depositor DCC
R_{free} test set	3132 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	72.4	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13999	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, EDO

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	0.47	0/3027	0.69	2/4114 (0.0%)
1	E	0.50	0/3122	0.68	1/4243 (0.0%)
2	B	0.37	0/863	0.70	0/1169
2	F	0.41	0/870	0.66	0/1179
3	C	0.54	1/1423 (0.1%)	0.79	1/1936 (0.1%)
3	G	0.47	0/1615	0.73	1/2197 (0.0%)
4	D	0.46	0/1659	0.74	2/2253 (0.1%)
4	H	0.44	0/1659	0.65	0/2253
All	All	0.47	1/14238 (0.0%)	0.70	7/19344 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	161	TRP	CG-CD1	-5.39	1.29	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	ARG	NE-CZ-NH2	-6.58	117.01	120.30
4	D	106	ILE	CG1-CB-CG2	-6.41	97.29	111.40
1	A	299	CYS	CA-CB-SG	6.08	124.95	114.00
1	E	76	ASP	CB-CG-OD1	5.69	123.42	118.30
4	D	139	PHE	C-N-CA	-5.33	108.37	121.70
3	G	172	THR	C-N-CA	-5.21	108.68	121.70
3	C	185	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2983	0	2904	55	1
1	E	3077	0	3010	47	0
2	B	844	0	826	29	0
2	F	851	0	835	21	0
3	C	1392	0	1354	51	0
3	G	1580	0	1544	42	1
4	D	1624	0	1581	61	0
4	H	1624	0	1581	43	0
5	A	4	0	6	0	0
5	E	4	0	6	0	0
6	A	6	0	8	1	0
6	E	6	0	8	1	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	H	2	0	0	0	0
All	All	13999	0	13663	325	1

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 (325) 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)
4:H:197:THR:HG22	4:H:204:PRO:HB3	1.37	1.06
1:A:215:THR:HG22	1:A:224:THR:HG22	1.40	1.03
3:C:38:ARG:HD3	3:C:48:ILE:HD11	1.53	0.89
3:G:142:THR:N	3:G:193:SER:HG	1.70	0.89
1:A:381:THR:HG21	2:F:76:LYS:HG3	1.55	0.86
1:A:213:THR:HG22	1:A:226:THR:HG22	1.60	0.84
1:E:174:LEU:HD12	1:E:174:LEU:H	1.43	0.83
4:D:189:HIS:O	4:D:211:ARG:NH1	2.13	0.82
1:E:329:GLU:OE2	1:E:331:SER:N	2.13	0.80
2:F:87:LYS:HG2	2:F:88:PRO:HD2	1.62	0.80
1:E:63:ARG:NH2	1:E:332:THR:O	2.15	0.79
3:C:147:CYS:SG	3:C:161:TRP:NE1	2.55	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:ARG:HG3	4:D:76:SER:HA	1.64	0.78
2:B:91:THR:HG22	2:B:113:VAL:H	1.49	0.78
1:E:202:THR:OG1	1:E:204:VAL:HG22	1.84	0.78
4:D:2:ILE:HD13	4:D:93:SER:HB3	1.65	0.77
4:D:61:ARG:NH1	4:D:82:ASP:OD2	2.20	0.75
4:D:140:TYR:O	4:D:142:ARG:N	2.20	0.74
3:C:153:PHE:H	3:C:154:PRO:HD2	1.52	0.74
3:C:62:ASP:OD1	3:C:65:LYS:NZ	2.15	0.73
4:H:108:ARG:HH12	4:H:111:ALA:HB2	1.55	0.71
3:G:82:GLN:HG3	3:G:84:ASN:ND2	2.06	0.71
1:A:343:ASN:OD1	1:A:346:THR:OG1	2.08	0.70
1:E:72:ASN:HA	1:E:76:ASP:OD2	1.90	0.70
2:B:39:ARG:HG2	2:B:94:TYR:HE1	1.56	0.69
4:D:161:GLU:HG3	4:D:175:LEU:HD21	1.74	0.69
4:D:70:ASP:C	4:D:71:PHE:HD1	1.96	0.69
1:E:321:GLN:NE2	1:E:363:LYS:HD3	2.07	0.68
3:C:188:VAL:HG21	4:D:135:LEU:HD11	1.75	0.68
3:G:82:GLN:HG3	3:G:84:ASN:HD21	1.59	0.68
4:D:198:HIS:HD2	4:D:199:GLN:H	1.41	0.68
2:B:49:VAL:HG13	2:B:64:VAL:HG21	1.75	0.67
3:C:131:LEU:HD21	3:C:148:LEU:HB2	1.75	0.67
4:H:120:PRO:HB2	4:H:125:LEU:HD11	1.77	0.66
2:B:91:THR:HA	2:B:112:THR:HA	1.78	0.66
3:G:108:ASP:OD2	3:G:109:HIS:ND1	2.27	0.66
2:B:60:TYR:HE1	2:B:70:ILE:HG22	1.61	0.65
2:F:67:ARG:NH1	2:F:85:SER:O	2.30	0.64
4:D:105:GLU:OE1	4:D:173:TYR:OH	2.14	0.64
1:E:171:LEU:HD13	1:E:262:LEU:HD12	1.80	0.64
4:D:37:GLN:HB2	4:D:47:LEU:HD11	1.81	0.63
4:H:155:GLN:HG3	4:H:179:LEU:HD11	1.80	0.63
2:B:86:LEU:HB3	2:B:113:VAL:HG21	1.80	0.63
3:G:5:VAL:HG22	3:G:23:GLU:CG	2.29	0.63
3:C:48:ILE:HG23	3:C:64:VAL:HG11	1.82	0.62
2:F:21:LEU:HD22	2:F:37:TRP:CH2	2.35	0.62
3:C:68:PHE:CZ	3:C:83:LEU:HD23	2.36	0.61
4:H:211:ARG:HG2	4:H:211:ARG:HH11	1.66	0.61
3:C:59:ARG:HE	4:D:94:THR:HG23	1.65	0.61
1:E:83:TYR:OH	1:E:171:LEU:O	2.17	0.61
4:D:151:ASP:OD2	4:D:189:HIS:ND1	2.33	0.61
4:D:24:ARG:NH1	4:D:70:ASP:OD1	2.34	0.61
1:A:166:ALA:HB1	1:A:262:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:HD2	4:D:32:TYR:CZ	2.36	0.60
1:A:312:ILE:O	1:A:316:GLN:HG3	2.02	0.60
1:E:52:LEU:HD11	2:F:45:LEU:HD21	1.84	0.60
1:E:220:GLY:O	1:E:221:LYS:HE2	2.02	0.60
1:E:242:ARG:HD2	4:H:32:TYR:CE2	2.37	0.59
1:E:438:ALA:HB2	2:F:34:VAL:HG11	1.84	0.59
1:A:215:THR:CG2	1:A:224:THR:HG22	2.25	0.59
3:C:1:GLN:O	3:C:1:GLN:NE2	2.36	0.59
3:C:147:CYS:SG	3:C:161:TRP:CD1	2.91	0.59
3:C:88:VAL:HA	3:C:118:VAL:HG22	1.84	0.59
3:C:129:PHE:HB3	4:D:121:SER:OG	2.03	0.59
3:C:161:TRP:HA	3:C:161:TRP:CE3	2.38	0.59
3:G:71:SER:HB2	3:G:80:PHE:HB2	1.85	0.59
1:A:112:GLY:O	1:A:142:PRO:HD2	2.02	0.58
4:D:122:ASP:HA	4:D:125:LEU:HD22	1.85	0.58
2:B:68:PHE:HB3	2:B:81:LEU:HD11	1.85	0.58
4:D:83:PHE:CD1	4:D:106:ILE:HG22	2.37	0.58
1:E:164:GLN:OE1	1:E:412:GLY:HA2	2.03	0.58
3:G:133:PRO:HG3	3:G:145:LEU:HB3	1.85	0.58
4:H:148:TRP:O	4:H:154:LEU:HA	2.02	0.58
1:A:230:LYS:NZ	1:A:247:GLU:OE2	2.31	0.58
3:G:29:PHE:CD2	3:G:77:GLU:HA	2.39	0.57
3:C:155:GLU:HB3	3:C:156:PRO:HD3	1.85	0.57
2:F:4:GLN:O	2:F:5:LEU:HD23	2.05	0.57
1:E:171:LEU:HD12	1:E:172:PRO:HD2	1.86	0.57
3:C:38:ARG:CD	3:C:48:ILE:HD11	2.32	0.57
4:D:198:HIS:CD2	4:D:199:GLN:H	2.22	0.57
1:A:453:ILE:O	1:A:457:LEU:HD13	2.05	0.56
3:G:8:GLY:HA3	3:G:114:THR:HG21	1.86	0.56
6:A:1002:GOL:H12	3:C:31:LEU:HD13	1.88	0.56
1:E:260:GLN:O	1:E:260:GLN:NE2	2.37	0.56
1:A:137:LEU:HD22	1:A:147:PRO:HG3	1.87	0.56
1:A:105:GLN:HE22	1:E:287:GLY:HA2	1.70	0.56
2:B:40:GLN:H	2:B:92:ALA:HB1	1.71	0.55
4:D:12:SER:HA	4:D:105:GLU:O	2.07	0.55
3:C:36:TRP:CE2	3:C:81:LEU:HB2	2.41	0.55
4:D:33:LEU:HD22	4:D:71:PHE:HD2	1.71	0.55
2:B:69:THR:HB	2:B:82:GLN:HG3	1.89	0.55
1:E:174:LEU:H	1:E:174:LEU:CD1	2.18	0.55
1:A:63:ARG:NH1	1:A:330:GLN:OE1	2.39	0.55
4:H:94:THR:HG23	4:H:95:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:CYS:HB3	2:B:79:LEU:HB3	1.88	0.55
1:A:105:GLN:HG2	1:A:147:PRO:HB3	1.89	0.54
3:C:188:VAL:HG11	4:D:135:LEU:HD13	1.89	0.54
4:H:124:GLN:HE21	4:H:129:THR:HG23	1.72	0.54
4:D:47:LEU:HA	4:D:58:VAL:HG21	1.88	0.54
3:G:32:PHE:O	3:G:72:ARG:NH2	2.40	0.54
1:E:163:LEU:HD21	1:E:265:GLN:HB2	1.89	0.54
1:A:66:LEU:HD21	1:A:358:ALA:HB2	1.90	0.53
3:C:68:PHE:CE2	3:C:83:LEU:HD23	2.43	0.53
2:F:21:LEU:HD21	2:F:109:THR:HG21	1.91	0.53
3:G:68:PHE:CE2	3:G:83:LEU:HD22	2.44	0.53
2:B:7:GLU:N	2:B:7:GLU:OE1	2.42	0.53
4:D:121:SER:O	4:D:125:LEU:HD13	2.08	0.53
3:G:5:VAL:HG22	3:G:23:GLU:HG3	1.89	0.53
3:G:52:GLY:O	3:G:72:ARG:NH1	2.42	0.53
4:D:83:PHE:CG	4:D:106:ILE:HG22	2.44	0.53
1:E:69:SER:OG	1:E:361:GLN:OE1	2.24	0.53
1:E:369:HIS:NE2	2:F:33:ASN:OD1	2.41	0.53
1:A:84:GLN:HB2	1:A:433:LEU:HD13	1.89	0.52
2:B:38:TYR:CD2	2:B:48:TRP:HA	2.44	0.52
1:E:141:LYS:HD3	1:E:142:PRO:O	2.09	0.52
4:H:170:ASP:HB3	4:H:172:THR:HG23	1.92	0.52
1:E:213:THR:HG23	1:E:226:THR:HG22	1.91	0.52
3:G:133:PRO:HG2	3:G:196:LEU:HD21	1.92	0.52
2:F:98:ARG:HG3	2:F:100:PRO:O	2.10	0.52
4:D:41:GLY:O	4:D:42:LYS:HE2	2.10	0.52
4:H:94:THR:HG23	4:H:95:LEU:CD1	2.40	0.52
3:G:6:GLN:OE1	3:G:113:GLY:N	2.40	0.52
4:D:14:SER:HB3	4:H:18:ARG:NH1	2.25	0.51
1:E:216:GLN:HG3	1:E:218:ILE:HD11	1.91	0.51
1:A:431:THR:OG1	2:B:55:GLN:NE2	2.44	0.51
3:G:133:PRO:HG2	3:G:196:LEU:CD2	2.41	0.51
4:H:155:GLN:HB3	4:H:158:ASN:HD21	1.76	0.51
1:A:438:ALA:HB2	2:B:34:VAL:HG21	1.92	0.50
3:C:191:VAL:HG13	3:C:192:PRO:HD2	1.94	0.50
4:D:120:PRO:HD3	4:D:132:VAL:HG22	1.93	0.50
4:H:175:LEU:HD23	4:H:176:SER:N	2.27	0.50
3:G:6:GLN:H	3:G:112:GLN:HE22	1.58	0.50
4:D:113:PRO:HD3	4:D:198:HIS:ND1	2.27	0.50
1:E:49:LEU:HD21	1:E:452:ASN:HB3	1.94	0.50
3:C:17:SER:HB3	3:C:84:ASN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:CYS:SG	1:E:397:ASN:ND2	2.85	0.49
3:C:188:VAL:HG21	4:D:135:LEU:CD1	2.41	0.49
2:F:87:LYS:CG	2:F:88:PRO:HD2	2.39	0.49
3:C:12:GLY:O	3:C:118:VAL:HA	2.12	0.49
1:A:206:ASP:OD2	3:C:30:ASN:ND2	2.46	0.49
1:E:321:GLN:HB2	1:E:364:MET:HG3	1.94	0.49
1:E:329:GLU:OE2	1:E:330:GLN:N	2.46	0.49
2:F:93:LEU:HD23	2:F:110:GLN:HA	1.94	0.49
3:C:151:ASP:HB3	3:C:182:LEU:HD22	1.95	0.49
4:D:198:HIS:CD2	4:D:199:GLN:N	2.81	0.49
1:A:273:ILE:HG23	1:A:298:LEU:HD13	1.95	0.48
2:B:5:LEU:O	2:B:6:GLN:HG3	2.13	0.48
4:D:175:LEU:HD23	4:D:176:SER:N	2.28	0.48
2:F:69:THR:HB	2:F:82:GLN:CG	2.44	0.48
3:C:159:VAL:HG21	3:C:172:THR:OG1	2.14	0.48
4:D:8:PRO:O	4:D:102:THR:OG1	2.23	0.48
1:A:63:ARG:HD2	1:A:330:GLN:OE1	2.14	0.48
1:A:208:ASN:ND2	3:C:53:SER:HB3	2.28	0.48
6:E:1002:GOL:H12	3:G:31:LEU:HD13	1.96	0.48
1:E:174:LEU:HD12	1:E:174:LEU:N	2.20	0.48
1:E:312:ILE:O	1:E:316:GLN:HG3	2.14	0.48
1:A:46:LEU:HD12	1:A:49:LEU:HB3	1.95	0.48
4:H:66:GLY:HA3	4:H:71:PHE:HA	1.96	0.48
4:H:90:GLN:HE22	4:H:93:SER:CB	2.27	0.47
3:C:2:VAL:HB	3:C:109:HIS:CD2	2.49	0.47
3:C:36:TRP:CG	3:C:81:LEU:HD22	2.49	0.47
1:E:334:VAL:HG21	1:E:350:PHE:CE1	2.49	0.47
2:B:83:MET:SD	2:B:94:TYR:HE2	2.38	0.47
1:E:310:LYS:NZ	1:E:314:ASP:OD2	2.39	0.47
2:F:60:TYR:CE1	2:F:70:ILE:HG22	2.49	0.47
3:G:68:PHE:CD1	3:G:83:LEU:HA	2.50	0.47
4:D:11:LEU:HD12	4:D:12:SER:N	2.29	0.47
1:A:310:LYS:NZ	1:A:314:ASP:OD1	2.47	0.47
3:C:2:VAL:HG13	3:C:27:PHE:CD1	2.50	0.47
1:A:289:PRO:HB2	1:A:391:PHE:CZ	2.49	0.47
1:A:379:ASN:ND2	2:B:31:SER:OG	2.47	0.47
3:C:64:VAL:HG21	3:C:68:PHE:CD2	2.50	0.47
4:H:33:LEU:HD13	4:H:71:PHE:CD2	2.49	0.47
4:H:147:GLN:HB2	4:H:195:GLU:HB3	1.96	0.47
4:D:91:SER:HA	4:D:96:TRP:CD1	2.50	0.47
3:G:6:GLN:HE22	3:G:95:PHE:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:LYS:HG2	2:F:88:PRO:CD	2.38	0.47
4:D:166:GLN:HG3	4:D:173:TYR:CZ	2.50	0.46
3:G:36:TRP:CZ3	3:G:96:CYS:HB3	2.51	0.46
4:D:106:ILE:HD13	4:D:106:ILE:HG21	1.70	0.46
1:E:83:TYR:HD2	1:E:84:GLN:NE2	2.13	0.46
3:C:131:LEU:HB3	4:D:118:PHE:CD2	2.51	0.46
1:A:188:THR:HA	1:A:246:THR:O	2.16	0.46
2:B:17:GLY:O	2:B:84:SER:HA	2.15	0.46
3:G:5:VAL:HG22	3:G:23:GLU:HG2	1.95	0.46
2:B:12:LEU:CD2	2:B:112:THR:OG1	2.64	0.46
4:H:154:LEU:HD23	4:H:155:GLN:O	2.16	0.46
4:H:37:GLN:HB2	4:H:47:LEU:HD11	1.97	0.46
4:D:14:SER:HB3	4:H:18:ARG:HH12	1.80	0.46
2:F:21:LEU:HD23	2:F:22:SER:H	1.79	0.46
2:B:23:CYS:HB2	2:B:37:TRP:CH2	2.51	0.46
4:D:71:PHE:N	4:D:71:PHE:CD1	2.84	0.46
1:A:304:GLU:OE1	1:A:304:GLU:N	2.46	0.46
3:C:100:ASN:HB2	3:C:108:ASP:HB2	1.97	0.46
4:H:211:ARG:HG2	4:H:211:ARG:NH1	2.31	0.46
2:F:69:THR:HB	2:F:82:GLN:HG3	1.97	0.45
3:G:44:SER:OG	3:G:45:LEU:N	2.49	0.45
4:H:150:VAL:HG12	4:H:192:TYR:CD2	2.50	0.45
1:A:211:THR:HG22	1:A:228:SER:HB3	1.98	0.45
4:H:166:GLN:HG3	4:H:173:TYR:CZ	2.52	0.45
1:A:454:ALA:O	1:A:458:VAL:HG23	2.16	0.45
4:D:190:LYS:HA	4:D:211:ARG:HD3	1.97	0.45
1:A:82:ALA:HB1	1:A:318:LEU:HD21	1.99	0.45
4:D:11:LEU:HD12	4:D:12:SER:H	1.81	0.45
1:A:395:CYS:SG	1:A:397:ASN:ND2	2.89	0.45
4:H:108:ARG:HB3	4:H:140:TYR:CD1	2.52	0.45
1:A:208:ASN:HD21	3:C:53:SER:CB	2.30	0.45
1:E:452:ASN:O	1:E:456:THR:HG23	2.17	0.45
3:C:153:PHE:N	3:C:154:PRO:HD2	2.26	0.45
4:D:47:LEU:O	4:D:48:ILE:HD13	2.17	0.45
1:E:317:GLU:OE2	1:E:321:GLN:NE2	2.50	0.45
2:B:86:LEU:HA	2:B:86:LEU:HD23	1.79	0.44
3:C:124:LYS:HE3	3:C:151:ASP:O	2.17	0.44
4:D:14:SER:HB2	4:D:17:ASP:OD2	2.17	0.44
4:D:71:PHE:HD1	4:D:71:PHE:N	2.14	0.44
2:B:12:LEU:HD23	2:B:112:THR:OG1	2.17	0.44
3:G:217:LYS:HG2	3:G:219:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:78:LEU:CD2	4:H:82:ASP:HB2	2.48	0.44
4:H:210:ASN:OD1	4:H:210:ASN:N	2.51	0.44
1:A:186:THR:HG22	1:A:249:THR:HA	1.99	0.44
3:G:146:GLY:HA2	3:G:161:TRP:CH2	2.52	0.44
1:A:70:ALA:HB2	1:A:361:GLN:NE2	2.33	0.44
4:D:167:ASP:HB3	4:D:170:ASP:HB2	2.00	0.44
2:B:18:SER:HA	2:B:83:MET:O	2.18	0.44
4:H:142:ARG:HB2	4:H:173:TYR:CE2	2.53	0.44
4:H:183:LYS:O	4:H:187:GLU:HG3	2.18	0.44
1:A:443:GLN:O	1:A:447:ILE:HG13	2.18	0.44
2:F:91:THR:HG22	2:F:113:VAL:N	2.32	0.44
4:D:73:LEU:HD23	4:D:74:THR:N	2.32	0.43
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.82	0.43
4:D:155:GLN:HG3	4:D:158:ASN:OD1	2.19	0.43
1:A:78:LYS:HG3	1:A:79:ASN:N	2.33	0.43
1:A:241:THR:O	1:A:243:VAL:HG23	2.18	0.43
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.90	0.43
3:C:87:ARG:NH2	3:C:89:ASP:OD2	2.48	0.43
4:D:125:LEU:O	4:D:183:LYS:HD3	2.19	0.43
4:H:150:VAL:HG22	4:H:155:GLN:OE1	2.19	0.43
2:B:29:ILE:HG22	2:B:35:MET:HE1	2.01	0.43
3:C:133:PRO:HB3	3:C:144:ALA:O	2.19	0.43
4:H:9:SER:O	4:H:102:THR:HA	2.19	0.43
1:A:223:VAL:HG22	1:A:254:GLY:O	2.18	0.43
3:G:98:ARG:HH21	3:G:100:ASN:ND2	2.17	0.43
4:H:145:LYS:O	4:H:196:VAL:HA	2.19	0.43
1:E:237:LYS:HE3	1:E:237:LYS:HB3	1.78	0.43
1:E:426:VAL:O	1:E:430:ILE:HG13	2.19	0.43
3:G:60:TYR:OH	3:G:69:ILE:HA	2.19	0.43
1:A:375:ILE:O	1:A:375:ILE:HG13	2.19	0.42
3:C:20:LEU:HD13	3:C:36:TRP:CZ3	2.54	0.42
4:D:139:PHE:HB2	4:D:198:HIS:HE1	1.84	0.42
2:F:64:VAL:HB	2:F:68:PHE:CD2	2.54	0.42
1:A:211:THR:HG22	1:A:228:SER:CB	2.49	0.42
2:B:71:SER:O	2:B:79:LEU:HD12	2.19	0.42
3:C:161:TRP:HA	3:C:161:TRP:HE3	1.82	0.42
1:E:169:LYS:HD2	1:E:181:VAL:HG23	2.01	0.42
4:D:141:PRO:HD2	4:D:198:HIS:NE2	2.34	0.42
3:G:98:ARG:HH21	3:G:100:ASN:HD22	1.66	0.42
3:G:100:ASN:HB2	3:G:108:ASP:HB2	2.00	0.42
3:G:36:TRP:CE2	3:G:81:LEU:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:43:GLN:OE1	3:G:43:GLN:HA	2.19	0.42
3:G:174:PRO:HG2	4:H:163:VAL:O	2.19	0.42
4:D:140:TYR:HB3	4:D:141:PRO:HD3	2.00	0.42
1:E:291:MET:HG3	1:E:292:GLU:N	2.35	0.42
3:C:153:PHE:O	3:C:154:PRO:C	2.58	0.42
1:A:91:ASN:HB3	1:A:424:ALA:HB1	2.01	0.42
4:D:139:PHE:HB2	4:D:198:HIS:CE1	2.55	0.42
3:C:20:LEU:HB2	3:C:81:LEU:HB3	2.01	0.42
4:H:107:LYS:HG2	4:H:108:ARG:N	2.35	0.42
3:C:67:ARG:CZ	3:C:87:ARG:HD3	2.49	0.42
4:D:69:THR:HG23	4:D:70:ASP:OD2	2.20	0.42
1:E:277:CYS:SG	1:E:297:LYS:HB2	2.60	0.42
4:D:84:ALA:O	4:D:104:VAL:HG22	2.19	0.41
1:E:267:SER:O	1:E:271:ASN:HB2	2.20	0.41
1:E:348:ALA:HA	1:E:350:PHE:CE1	2.54	0.41
3:G:7:SER:HB2	3:G:21:ALA:HB3	2.02	0.41
1:A:242:ARG:HD2	4:D:32:TYR:CE2	2.54	0.41
3:C:29:PHE:CD2	3:C:77:GLU:HA	2.55	0.41
1:E:212:LYS:HE3	1:E:214:LYS:HG3	2.02	0.41
4:H:6:GLN:H	4:H:100:GLN:HE22	1.68	0.41
4:D:70:ASP:C	4:D:71:PHE:CD1	2.86	0.41
3:G:86:LEU:HB3	3:G:118:VAL:HG11	2.02	0.41
1:A:68:ALA:O	1:A:72:ASN:HB2	2.20	0.41
2:B:73:ASP:CG	2:B:76:LYS:HB2	2.41	0.41
3:C:20:LEU:HD12	3:C:81:LEU:HD23	2.01	0.41
3:C:83:LEU:HB3	3:C:86:LEU:HD21	2.02	0.41
4:D:108:ARG:HG2	4:D:109:THR:N	2.35	0.41
4:D:155:GLN:HG2	4:D:179:LEU:HD11	2.03	0.41
1:E:139:ARG:HE	1:E:139:ARG:HB3	1.71	0.41
1:E:304:GLU:OE2	1:E:304:GLU:N	2.49	0.41
3:G:67:ARG:O	3:G:68:PHE:HD1	2.04	0.41
4:H:148:TRP:CE3	4:H:179:LEU:HD12	2.56	0.41
1:A:87:LEU:HD12	1:A:87:LEU:HA	1.91	0.41
2:B:67:ARG:HD2	2:B:85:SER:HB3	2.03	0.41
3:C:173:PHE:O	3:C:185:LEU:HG	2.20	0.41
4:H:148:TRP:O	4:H:154:LEU:HG	2.21	0.41
1:A:459:ASN:O	1:A:463:HIS:ND1	2.54	0.41
3:C:88:VAL:HA	3:C:118:VAL:CG2	2.51	0.41
4:D:106:ILE:H	4:D:106:ILE:HG23	1.65	0.41
3:G:18:LEU:HB2	3:G:83:LEU:HD12	2.03	0.41
4:H:106:ILE:HG22	4:H:166:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:140:TYR:O	4:H:142:ARG:N	2.54	0.41
2:B:5:LEU:HD21	2:B:96:CYS:SG	2.60	0.41
3:C:98:ARG:HH21	3:C:100:ASN:HD22	1.69	0.41
1:E:66:LEU:HD23	1:E:66:LEU:HA	1.91	0.41
3:G:32:PHE:CE2	3:G:102:TRP:HD1	2.39	0.41
3:G:38:ARG:NE	3:G:48:ILE:HD11	2.36	0.41
3:G:16:GLY:O	3:G:86:LEU:HD12	2.20	0.41
3:G:157:VAL:HG22	3:G:207:HIS:HD2	1.85	0.41
1:A:445:GLN:HA	1:A:445:GLN:OE1	2.20	0.40
2:F:38:TYR:CD1	2:F:48:TRP:HA	2.56	0.40
4:H:166:GLN:HG3	4:H:173:TYR:CE1	2.56	0.40
4:D:118:PHE:HA	4:D:119:PRO:HD3	1.93	0.40
3:G:149:VAL:CG2	3:G:185:LEU:HB3	2.50	0.40
4:H:145:LYS:HB3	4:H:197:THR:OG1	2.22	0.40
1:A:66:LEU:HD12	1:A:66:LEU:HA	1.89	0.40
1:A:397:ASN:HD22	1:A:409:SER:HB2	1.85	0.40
1:E:88:LEU:HD13	1:E:429:THR:HG22	2.04	0.40
1:A:308:ILE:HA	1:A:311:MET:HE3	2.04	0.40
3:C:107:LEU:HA	3:C:107:LEU:HD23	1.82	0.40
4:H:46:LEU:HD23	4:H:55:GLN:HE21	1.86	0.40
1:A:242:ARG:HH21	1:A:242:ARG:HG2	1.85	0.40
1:A:442:THR:HG23	2:B:48:TRP:CE3	2.57	0.40
1:E:125:GLU:OE2	1:E:157:ASN:ND2	2.35	0.40
2:F:39:ARG:HB2	2:F:92:ALA:HB3	2.03	0.40
3:G:6:GLN:NE2	3:G:96:CYS:H	2.20	0.40
4:H:90:GLN:HE22	4:H:93:SER:HB3	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:NH2	3:G:14:PRO:O[2_555]	1.91	0.29

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	393/466 (84%)	374 (95%)	19 (5%)	0	100	100
1	E	407/466 (87%)	387 (95%)	19 (5%)	1 (0%)	47	73
2	B	108/120 (90%)	102 (94%)	6 (6%)	0	100	100
2	F	109/120 (91%)	107 (98%)	2 (2%)	0	100	100
3	C	185/222 (83%)	162 (88%)	17 (9%)	6 (3%)	4	9
3	G	209/222 (94%)	186 (89%)	20 (10%)	3 (1%)	11	28
4	D	209/211 (99%)	195 (93%)	12 (6%)	2 (1%)	15	37
4	H	209/211 (99%)	193 (92%)	15 (7%)	1 (0%)	29	54
All	All	1829/2038 (90%)	1706 (93%)	110 (6%)	13 (1%)	22	46

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	155	GLU
3	C	192	PRO
4	D	141	PRO
3	G	8	GLY
4	H	8	PRO
4	D	140	TYR
3	G	41	PRO
3	G	54	SER
3	C	153	PHE
1	E	129	ARG
3	C	41	PRO
3	C	154	PRO
3	C	191	VAL

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	331/381 (87%)	323 (98%)	8 (2%)	49 77
1	E	342/381 (90%)	336 (98%)	6 (2%)	59 83
2	B	89/99 (90%)	86 (97%)	3 (3%)	37 66
2	F	90/99 (91%)	87 (97%)	3 (3%)	38 67
3	C	153/182 (84%)	145 (95%)	8 (5%)	23 49
3	G	175/182 (96%)	172 (98%)	3 (2%)	60 84
4	D	187/187 (100%)	186 (100%)	1 (0%)	88 96
4	H	187/187 (100%)	180 (96%)	7 (4%)	34 63
All	All	1554/1698 (92%)	1515 (98%)	39 (2%)	47 76

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

Mol	Chain	Res	Type
1	A	66	LEU
1	A	111	ASN
1	A	137	LEU
1	A	145	TYR
1	A	182	SER
1	A	252	LEU
1	A	282	VAL
1	A	347	ASP
2	B	21	LEU
2	B	28	SER
2	B	39	ARG
3	C	25	SER
3	C	58	THR
3	C	108	ASP
3	C	114	THR
3	C	118	VAL
3	C	119	SER
3	C	159	VAL
3	C	160	SER
4	D	71	PHE
1	E	140	TYR
1	E	145	TYR
1	E	151	GLU
1	E	292	GLU
1	E	320	ASN
1	E	329	GLU
2	F	21	LEU

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Mol	Chain	Res	Type
2	F	96	CYS
2	F	112	THR
3	G	25	SER
3	G	71	SER
3	G	72	ARG
4	H	3	GLN
4	H	9	SER
4	H	61	ARG
4	H	81	GLU
4	H	90	GLN
4	H	136	LEU
4	H	147	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	A	379	ASN
1	A	397	ASN
2	B	33	ASN
3	C	1	GLN
4	D	124	GLN
4	D	198	HIS
1	E	207	GLN
1	E	321	GLN
1	E	386	ASN
2	F	82	GLN
3	G	84	ASN
4	H	6	GLN
4	H	124	GLN
4	H	147	GLN
4	H	155	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	EDO	E	1001	-	3,3,3	0.71	0	2,2,2	0.42	0
6	GOL	E	1002	-	5,5,5	0.87	0	5,5,5	1.14	0
6	GOL	A	1002	-	5,5,5	1.12	0	5,5,5	1.00	0
5	EDO	A	1001	-	3,3,3	0.62	0	2,2,2	0.06	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	EDO	E	1001	-	-	1/1/1/1	-
6	GOL	E	1002	-	-	2/4/4/4	-
6	GOL	A	1002	-	-	2/4/4/4	-
5	EDO	A	1001	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	GOL	C1-C2-C3-O3
6	E	1002	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	1002	GOL	O2-C2-C3-O3
6	E	1002	GOL	O2-C2-C3-O3
5	A	1001	EDO	O1-C1-C2-O2
5	E	1001	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1002	GOL	1	0
6	A	1002	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	401/466 (86%)	-0.02	4 (0%) 82 83	57, 88, 129, 157	0
1	E	413/466 (88%)	-0.04	8 (1%) 66 69	62, 84, 136, 171	0
2	B	110/120 (91%)	0.73	13 (11%) 4 3	112, 150, 165, 182	0
2	F	111/120 (92%)	0.18	5 (4%) 33 31	82, 111, 142, 167	0
3	C	189/222 (85%)	0.05	8 (4%) 36 35	70, 99, 152, 170	0
3	G	213/222 (95%)	-0.03	4 (1%) 66 69	75, 95, 117, 125	0
4	D	211/211 (100%)	0.09	7 (3%) 46 46	70, 106, 142, 153	0
4	H	211/211 (100%)	-0.02	3 (1%) 75 77	79, 116, 140, 154	0
All	All	1859/2038 (91%)	0.05	52 (2%) 53 54	57, 97, 149, 182	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	42	ARG	6.2
2	F	103	ARG	6.1
3	C	128	VAL	5.7
4	D	184	ALA	4.1
1	E	39	LEU	3.7
2	B	18	SER	3.7
2	B	25	ALA	3.5
2	F	16	GLY	3.4
2	B	17	GLY	3.4
4	D	190	LYS	3.3
3	C	166	LEU	3.2
3	G	143	ALA	3.2
2	B	11	GLY	3.2
3	C	126	PRO	3.1
1	E	36	LEU	3.0
2	B	40	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	208	SER	2.9
2	F	21	LEU	2.9
2	B	27	GLY	2.9
2	B	79	LEU	2.9
2	B	95	TYR	2.9
2	B	19	LEU	2.8
4	H	115	VAL	2.8
3	C	86	LEU	2.7
3	C	119	SER	2.7
2	B	6	GLN	2.7
3	C	11	ILE	2.7
1	A	339	GLY	2.6
2	B	45	LEU	2.5
3	C	129	PHE	2.5
1	E	348	ALA	2.4
3	C	191	VAL	2.4
3	G	152	TYR	2.3
2	B	84	SER	2.3
3	G	10	GLY	2.3
1	A	54	ALA	2.3
1	E	38	LYS	2.3
2	B	66	GLY	2.2
4	D	92	TYR	2.2
1	E	353	GLY	2.2
4	D	154	LEU	2.2
1	E	54	ALA	2.2
1	A	50	ILE	2.2
2	F	68	PHE	2.1
4	D	133	VAL	2.1
4	D	116	PHE	2.1
4	H	47	LEU	2.1
1	E	43	TYR	2.0
4	H	24	ARG	2.0
3	G	155	GLU	2.0
2	F	84	SER	2.0
1	A	51	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
5	EDO	E	1001	4/4	0.87	0.21	68,71,74,79	0
6	GOL	A	1002	6/6	0.91	0.30	80,82,85,86	0
5	EDO	A	1001	4/4	0.94	0.18	78,79,79,83	0
6	GOL	E	1002	6/6	0.94	0.20	83,85,85,87	0

6.5 Other polymers (i)

There are no such residues in this entry.