



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 3QEH / pdb_00003qeh
Title : Crystal structure of human N12-i15, an ADCC and non-neutralizing anti-HIV-1 Env antibody
Authors : Guan, Y.; DeVico, A.L.; Lewis, G.K.; Pazgier, M.
Deposited on : 2011-01-20
Resolution : 2.59 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

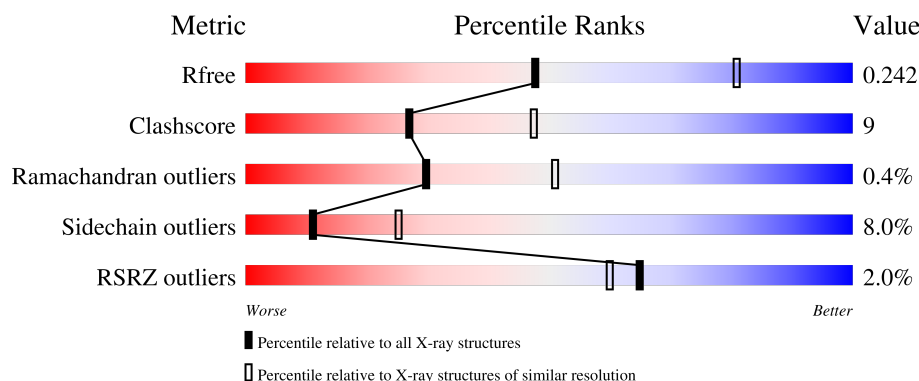
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	232	 2% 73% 17% • 7%
1	C	232	 % 73% 16% • 8%
1	E	232	 2% 72% 15% • 8%
1	G	232	 5% 63% 17% • 17%
2	B	218	 74% 21% ••

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Mol	Chain	Length	Quality of chain
2	D	218	78% 19% ..
2	F	218	% 78% 18% . .
2	H	218	3% 59% 25% 5% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13446 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.

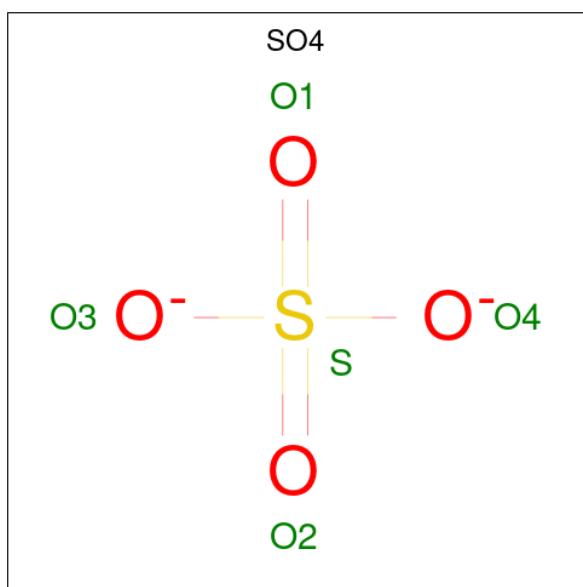
- Molecule 1 is a protein called Fab fragment of human anti-HIV-1 Env antibody N12-i15, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1649	1043	281	318	7			
1	C	213	Total	C	N	O	S	0	0	0
			1630	1031	278	314	7			
1	E	214	Total	C	N	O	S	0	0	0
			1638	1037	279	315	7			
1	G	192	Total	C	N	O	S	0	0	0
			1475	939	250	279	7			

- Molecule 2 is a protein called Fab fragment of human anti-HIV-1 Env antibody N12-i15, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1655	1038	280	331	6			
2	D	215	Total	C	N	O	S	0	0	0
			1655	1038	280	331	6			
2	F	212	Total	C	N	O	S	0	0	0
			1631	1023	276	326	6			
2	H	193	Total	C	N	O	S	0	0	0
			1498	941	254	297	6			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	3	Total	Cl	0	0
			3	3		
4	C	2	Total	Cl	0	0
			2	2		
4	D	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

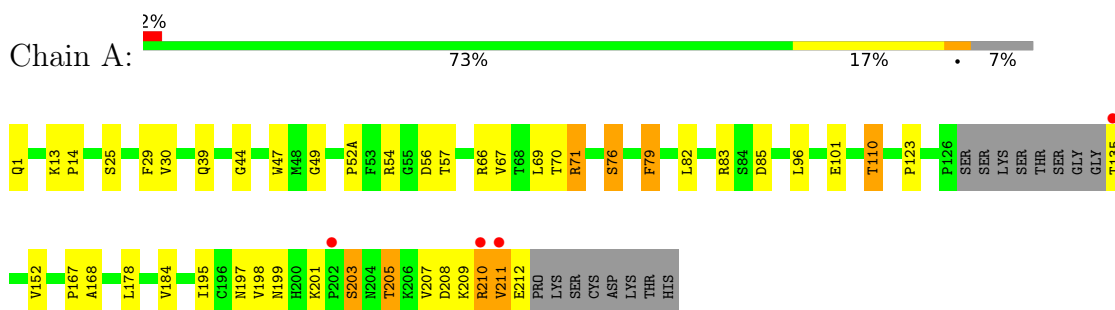
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	104	Total	O	0	0
			104	104		
6	B	78	Total	O	0	0
			78	78		
6	C	75	Total	O	0	0
			75	75		
6	D	82	Total	O	0	0
			82	82		
6	E	64	Total	O	0	0
			64	64		
6	F	63	Total	O	0	0
			63	63		
6	G	63	Total	O	0	0
			63	63		
6	H	37	Total	O	0	0
			37	37		

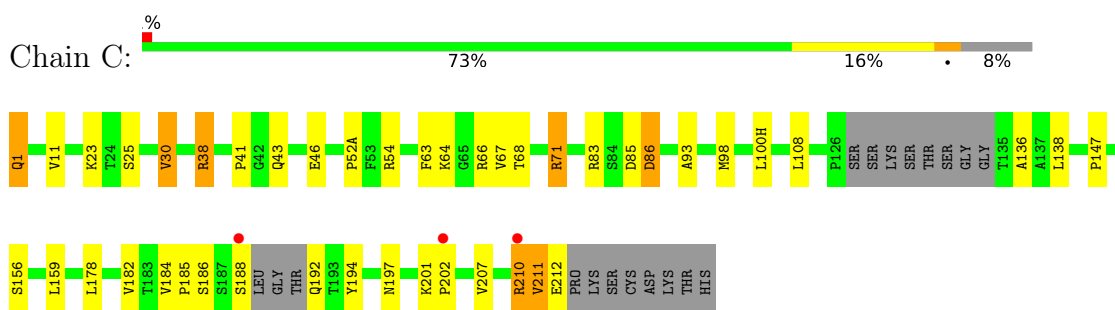
3 Residue-property plots [i](#)

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.

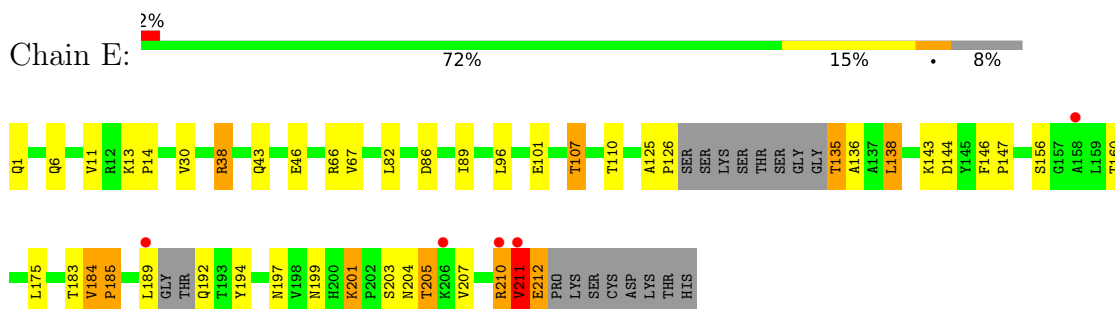
- Molecule 1: Fab fragment of human anti-HIV-1 Env antibody N12-i15, heavy chain



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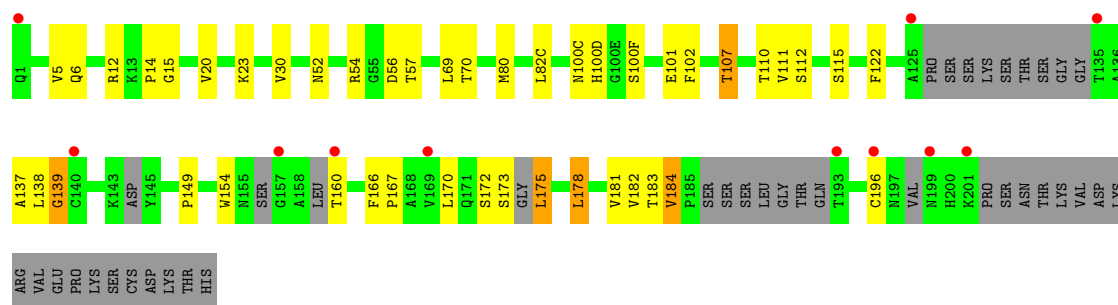


- Molecule 1: Fab fragment of human anti-HIV-1 Env antibody N12-i15, heavy chain



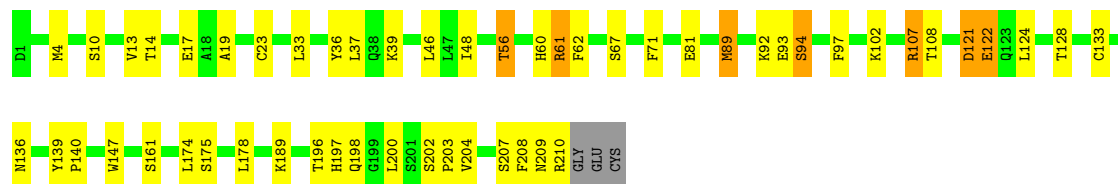
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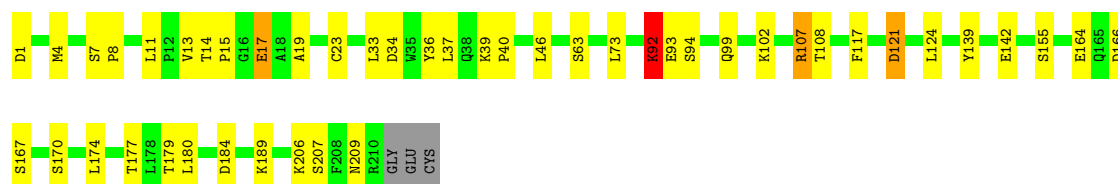
- Molecule 2: Fab fragment of human anti-HIV-1 Env antibody N12-i15,light chain

Chain B: 74% 21% ..



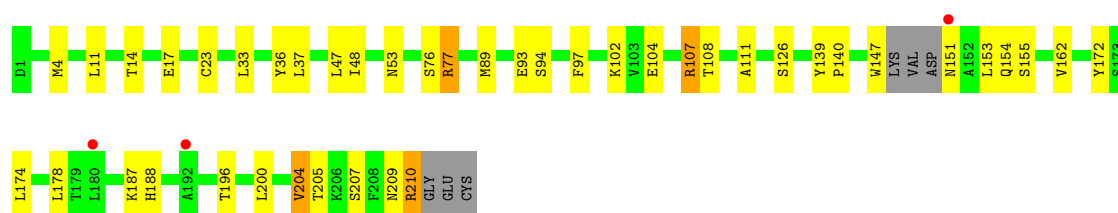
- Molecule 2: Fab fragment of human anti-HIV-1 Env antibody N12-i15,light chain

Chain D: 78% 19% ..



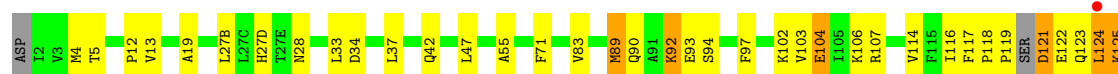
- Molecule 2: Fab fragment of human anti-HIV-1 Env antibody N12-i15,light chain

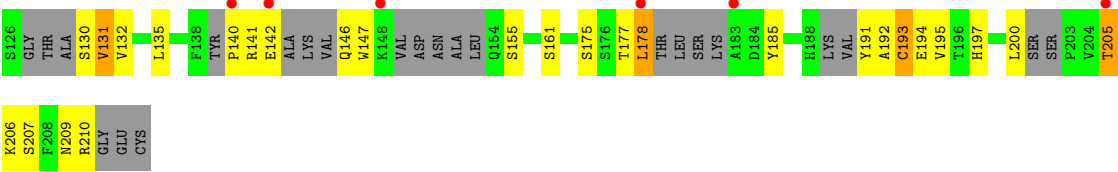
Chain F: 78% 18% ..



- Molecule 2: Fab fragment of human anti-HIV-1 Env antibody N12-i15,light chain

Chain H: 3% 59% 25% 5% 11%





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	125.12Å 125.12Å 149.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.59 20.00 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.59) 99.5 (20.00-2.59)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.216 , 0.254 0.199 , 0.242	Depositor DCC
R_{free} test set	3615 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
Reported twinning fraction	0.941 for H, K, L 0.059 for K, H, -L	Depositor
Outliers	1 of 71531 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13446	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6355e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, 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	1.13	2/1688 (0.1%)	1.10	2/2299 (0.1%)
1	C	1.13	1/1668 (0.1%)	1.13	1/2270 (0.0%)
1	E	1.01	0/1676	1.07	1/2281 (0.0%)
1	G	0.99	1/1506 (0.1%)	1.02	4/2042 (0.2%)
2	B	1.06	0/1691	1.14	8/2295 (0.3%)
2	D	1.07	0/1691	1.14	5/2295 (0.2%)
2	F	1.01	0/1666	1.06	4/2260 (0.2%)
2	H	0.95	1/1525 (0.1%)	1.09	4/2055 (0.2%)
All	All	1.05	5/13111 (0.0%)	1.10	29/17797 (0.2%)

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
1	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	5	VAL	CA-CB	7.02	1.62	1.54
1	A	79	PHE	CA-C	-6.39	1.44	1.52
1	A	168	ALA	CA-CB	-5.67	1.44	1.53
2	H	55	ALA	CA-CB	-5.23	1.45	1.53
1	C	98	MET	N-CA	5.21	1.52	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	117	PHE	CA-C-N	8.43	125.81	119.66
2	D	117	PHE	C-N-CA	8.43	125.81	119.66
1	G	139	GLY	N-CA-C	7.42	120.56	110.69
2	B	94	SER	CA-C-N	-7.15	112.63	119.85
2	B	94	SER	C-N-CA	-7.15	112.63	119.85
1	A	201	LYS	N-CA-C	-7.15	100.64	109.65
2	B	121	ASP	CA-C-N	6.55	128.96	120.44
2	B	121	ASP	C-N-CA	6.55	128.96	120.44
2	D	92	LYS	N-CA-C	-6.53	103.66	111.69
2	D	207	SER	N-CA-C	6.36	118.61	109.14
1	C	86	ASP	N-CA-C	-6.26	105.22	112.92
2	F	111	ALA	CA-C-N	-5.85	114.24	120.03
2	F	111	ALA	C-N-CA	-5.85	114.24	120.03
2	H	118	PRO	O-C-N	5.81	123.88	121.15
2	B	92	LYS	N-CA-C	-5.74	104.40	111.40
2	H	92	LYS	N-CA-C	-5.70	104.98	111.14
2	D	177	THR	CB-CA-C	-5.67	101.08	110.14
2	H	177	THR	N-CA-C	5.59	117.75	108.13
1	G	100(F)	SER	N-CA-C	5.56	118.14	110.35
2	B	136	ASN	N-CA-C	5.51	118.46	109.59
1	G	12	ARG	N-CA-C	5.37	117.93	108.75
2	F	155	SER	N-CA-C	5.35	118.17	109.24
2	H	114	VAL	N-CA-C	5.30	115.59	108.17
1	A	208	ASP	N-CA-C	5.19	117.53	108.76
2	B	207	SER	N-CA-C	5.17	116.84	109.14
2	B	200	LEU	N-CA-C	5.12	116.87	108.52
1	E	43	GLN	N-CA-C	5.06	117.54	109.65
1	G	15	GLY	N-CA-C	-5.04	108.69	114.69
2	F	207	SER	N-CA-C	5.04	116.84	109.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	SER	Peptide
1	E	211	VAL	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	1649	0	1615	35	0
1	C	1630	0	1593	27	0
1	E	1638	0	1604	29	0
1	G	1475	0	1434	29	0
2	B	1655	0	1620	35	0
2	D	1655	0	1620	22	0
2	F	1631	0	1593	21	0
2	H	1498	0	1448	39	0
3	A	5	0	0	0	0
3	E	5	0	0	0	0
3	G	5	0	0	1	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	1
4	H	1	0	0	0	0
5	D	6	0	8	0	0
5	E	6	0	8	0	0
5	F	6	0	8	0	0
5	H	6	0	8	0	0
6	A	104	0	0	6	0
6	B	78	0	0	1	0
6	C	75	0	0	3	0
6	D	82	0	0	2	0
6	E	64	0	0	1	2
6	F	63	0	0	0	3
6	G	63	0	0	0	0
6	H	37	0	0	1	0
All	All	13446	0	12559	233	3

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 9.

All (233) 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:210:ARG:O	1:E:210:ARG:HD3	1.41	1.20
2:H:141:ARG:O	2:H:141:ARG:HG2	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:ASN:OD1	1:E:205:THR:HG22	1.66	0.95
1:G:166:PHE:O	1:G:178:LEU:HD21	1.67	0.95
1:G:170:LEU:HD11	1:G:175:LEU:HD13	1.49	0.94
1:C:138:LEU:HD13	1:C:210:ARG:HD2	1.52	0.90
1:A:210:ARG:HA	1:A:210:ARG:NE	1.88	0.88
2:F:89:MET:HE2	2:F:97:PHE:CZ	2.12	0.85
1:E:210:ARG:O	1:E:210:ARG:CD	2.25	0.83
1:A:123:PRO:HB3	1:A:210:ARG:HD3	1.61	0.81
2:H:89:MET:HE3	2:H:97:PHE:CZ	2.16	0.80
1:G:173:SER:C	1:G:175:LEU:HD23	2.07	0.80
1:A:123:PRO:CB	1:A:210:ARG:HD3	2.12	0.79
2:H:141:ARG:O	2:H:141:ARG:CG	2.30	0.79
1:C:1:GLN:CD	1:C:1:GLN:N	2.42	0.78
2:D:11:LEU:HD21	2:D:19:ALA:HB1	1.65	0.78
1:A:199:ASN:OD1	1:A:205:THR:HG22	1.83	0.78
2:B:189:LYS:HZ3	2:B:210:ARG:HA	1.49	0.75
2:D:107:ARG:HD3	2:D:108:THR:O	1.86	0.75
2:H:147:TRP:CD2	2:H:178:LEU:HD11	2.24	0.73
2:D:99:GLN:HG2	6:D:419:HOH:O	1.87	0.73
1:E:6:GLN:HE21	1:E:107:THR:HG23	1.54	0.72
2:F:151:ASN:OD1	2:F:151:ASN:O	2.08	0.72
2:B:189:LYS:NZ	2:B:210:ARG:HA	2.04	0.72
1:A:83:ARG:HG3	1:A:85:ASP:OD1	1.90	0.71
1:E:38:ARG:HD2	1:E:46:GLU:OE1	1.91	0.71
2:H:178:LEU:HD12	2:H:178:LEU:H	1.53	0.71
1:C:83:ARG:HG3	1:C:85:ASP:OD1	1.91	0.70
1:A:110:THR:CG2	6:A:245:HOH:O	2.40	0.68
1:E:6:GLN:NE2	1:E:107:THR:HG23	2.08	0.68
1:C:52(A):PRO:O	1:C:71:ARG:HD2	1.95	0.67
2:H:140:PRO:HD2	2:H:197:HIS:CE1	2.29	0.67
2:D:189:LYS:HD2	2:D:209:ASN:HB3	1.77	0.67
1:A:211:VAL:O	1:A:212:GLU:HB2	1.95	0.66
1:A:167:PRO:HG2	2:B:161:SER:HB2	1.77	0.66
2:B:107:ARG:HD3	2:B:108:THR:O	1.95	0.66
1:A:25:SER:HB3	1:C:25:SER:HB3	1.77	0.66
2:B:89:MET:HE3	2:B:97:PHE:CZ	2.31	0.65
2:D:166:ASP:O	2:D:170:SER:HA	1.96	0.65
1:A:70:THR:HG22	1:A:79:PHE:HB2	1.79	0.64
1:A:210:ARG:HA	1:A:210:ARG:CZ	2.28	0.64
1:E:96:LEU:HD12	1:E:101:GLU:OE1	1.98	0.64
1:A:123:PRO:HB3	1:A:210:ARG:CD	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:SER:C	1:G:175:LEU:CD2	2.72	0.62
1:C:66:ARG:NH2	1:C:86:ASP:OD2	2.34	0.61
2:B:89:MET:CE	2:B:97:PHE:CZ	2.84	0.61
2:F:107:ARG:CD	2:F:108:THR:O	2.49	0.61
1:A:39:GLN:HG3	1:A:44:GLY:O	2.01	0.60
2:B:174:LEU:C	2:B:174:LEU:HD23	2.26	0.60
1:E:210:ARG:O	1:E:210:ARG:NH1	2.30	0.60
1:A:209:LYS:O	1:A:210:ARG:HD2	2.02	0.59
2:F:107:ARG:HD3	2:F:108:THR:O	2.01	0.59
2:F:36:TYR:CE1	2:F:89:MET:HE3	2.37	0.59
2:H:178:LEU:HD12	2:H:178:LEU:N	2.18	0.59
2:B:4:MET:HE3	2:B:23:CYS:SG	2.43	0.59
1:A:210:ARG:NE	1:A:210:ARG:CA	2.65	0.58
2:B:14:THR:HB	2:B:17:GLU:HG3	1.84	0.58
2:H:147:TRP:CE2	2:H:178:LEU:HD11	2.39	0.58
2:F:209:ASN:O	2:F:210:ARG:NE	2.29	0.58
2:F:147:TRP:HB2	2:F:154:GLN:HB2	1.86	0.57
2:B:121:ASP:HB2	2:B:122:GLU:OE1	2.05	0.57
1:C:1:GLN:CD	1:C:1:GLN:H1	2.11	0.57
2:H:27(B):LEU:HD22	2:H:90:GLN:HG2	1.86	0.57
2:H:12:PRO:HB2	2:H:106:LYS:HB2	1.87	0.57
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.40	0.57
1:E:194:TYR:HB2	1:E:210:ARG:HD2	1.87	0.57
2:H:33:LEU:HD22	2:H:71:PHE:CG	2.40	0.57
2:B:93:GLU:O	2:B:94:SER:C	2.48	0.56
2:H:119:PRO:HB3	2:H:130:SER:N	2.19	0.56
2:H:4:MET:SD	2:H:90:GLN:HB2	2.46	0.56
1:C:211:VAL:O	1:C:212:GLU:HB2	2.05	0.56
1:G:54:ARG:HB2	1:G:56:ASP:OD1	2.06	0.56
1:C:136:ALA:HB2	1:C:186:SER:HB3	1.88	0.56
1:E:210:ARG:HD3	1:E:210:ARG:C	2.23	0.56
2:F:14:THR:HB	2:F:17:GLU:OE1	2.06	0.55
1:C:1:GLN:N	1:C:1:GLN:OE1	2.34	0.55
2:D:33:LEU:HG	2:D:34:ASP:N	2.22	0.55
2:H:119:PRO:O	2:H:121:ASP:N	2.39	0.55
2:H:209:ASN:O	2:H:210:ARG:HB2	2.07	0.55
2:H:124:LEU:HD22	2:H:125:LYS:HB3	1.88	0.54
1:A:70:THR:CG2	1:A:79:PHE:HB2	2.38	0.54
2:B:39:LYS:NZ	2:B:81:GLU:OE1	2.35	0.54
1:C:194:TYR:HB2	1:C:210:ARG:HH11	1.73	0.54
1:C:210:ARG:NH2	1:C:212:GLU:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:PRO:HG2	2:H:161:SER:HB2	1.91	0.53
2:D:13:VAL:HG21	2:D:19:ALA:HB2	1.90	0.53
1:G:6:GLN:HE21	1:G:107:THR:CG2	2.21	0.53
1:A:71:ARG:O	1:A:71:ARG:HG2	2.08	0.53
1:C:210:ARG:O	1:C:210:ARG:CZ	2.56	0.53
2:H:140:PRO:HD2	2:H:197:HIS:HE1	1.71	0.53
2:F:93:GLU:O	2:F:94:SER:C	2.50	0.53
2:H:146:GLN:HB2	2:H:194:GLU:HB3	1.90	0.52
1:G:139:GLY:HA2	1:G:154:TRP:CH2	2.45	0.52
2:H:12:PRO:HB3	2:H:104:GLU:OE2	2.10	0.52
1:C:66:ARG:HH22	1:C:86:ASP:CG	2.17	0.52
2:H:185:TYR:HA	2:H:191:TYR:OH	2.09	0.52
1:A:96:LEU:HD12	1:A:101:GLU:OE1	2.10	0.51
2:B:202:SER:HB2	2:B:203:PRO:HD2	1.92	0.51
1:G:6:GLN:HE21	1:G:107:THR:HG23	1.75	0.51
2:H:193:CYS:N	2:H:206:LYS:O	2.37	0.51
1:A:57:THR:HG21	1:A:69:LEU:HB2	1.92	0.51
1:C:38:ARG:NH1	1:C:46:GLU:OE1	2.44	0.51
1:E:184:VAL:HG22	1:E:185:PRO:HD2	1.93	0.51
2:D:36:TYR:CE2	2:D:46:LEU:HD13	2.46	0.51
1:A:67:VAL:HG22	1:A:82:LEU:HD13	1.93	0.50
1:A:152:VAL:HG22	1:A:198:VAL:HG22	1.94	0.50
1:E:11:VAL:HG21	1:E:147:PRO:HG3	1.94	0.50
2:F:4:MET:HE3	2:F:23:CYS:SG	2.52	0.50
1:E:66:ARG:NH2	1:E:86:ASP:OD2	2.40	0.50
2:D:11:LEU:CD2	2:D:19:ALA:HB1	2.39	0.50
2:B:36:TYR:CE2	2:B:46:LEU:HD13	2.47	0.50
2:B:89:MET:HE3	2:B:97:PHE:CE2	2.47	0.49
1:A:210:ARG:CZ	1:A:211:VAL:H	2.25	0.49
1:G:14:PRO:HD3	1:G:112:SER:C	2.37	0.49
2:H:192:ALA:HA	2:H:207:SER:HB3	1.94	0.49
1:G:82(C):LEU:HD13	1:G:111:VAL:HG22	1.93	0.49
1:E:96:LEU:HD12	1:E:101:GLU:CD	2.38	0.49
2:H:83:VAL:HG13	2:H:103:VAL:O	2.13	0.49
1:C:41:PRO:HA	6:C:371:HOH:O	2.13	0.49
2:D:92:LYS:NZ	6:D:348:HOH:O	2.45	0.49
1:G:52:ASN:ND2	3:G:221:SO4:O2	2.44	0.49
1:A:110:THR:HG23	6:A:245:HOH:O	2.07	0.49
2:B:208:PHE:C	2:B:208:PHE:CD2	2.91	0.49
1:C:93:ALA:HB1	1:C:100(H):LEU:HB3	1.95	0.48
2:H:124:LEU:HA	2:H:125:LYS:HA	1.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52(A):PRO:O	1:A:71:ARG:HD2	2.12	0.48
2:B:210:ARG:HB2	6:B:392:HOH:O	2.14	0.48
1:E:197:ASN:HD22	1:E:207:VAL:HG22	1.79	0.48
2:B:67:SER:HA	2:B:71:PHE:CE1	2.49	0.48
1:C:11:VAL:HG21	1:C:147:PRO:HG3	1.96	0.47
1:C:63:PHE:O	1:C:67:VAL:HG12	2.13	0.47
2:F:107:ARG:HD2	2:F:108:THR:O	2.14	0.47
1:E:6:GLN:HB3	1:E:107:THR:CG2	2.44	0.47
2:H:197:HIS:H	2:H:200:LEU:HD12	1.80	0.47
1:C:184:VAL:HG11	1:C:194:TYR:OH	2.14	0.47
2:D:107:ARG:HD2	2:D:139:TYR:HB3	1.97	0.47
1:C:184:VAL:HG12	1:C:185:PRO:O	2.15	0.47
1:G:137:ALA:HB2	1:G:183:THR:HG22	1.97	0.47
1:A:96:LEU:HD12	1:A:101:GLU:CD	2.40	0.46
1:G:139:GLY:HA2	1:G:154:TRP:HH2	1.81	0.46
6:A:223:HOH:O	2:B:56:THR:HG23	2.15	0.46
2:F:104:GLU:OE2	2:F:172:TYR:OH	2.25	0.46
2:H:121:ASP:OD2	2:H:122:GLU:HG2	2.15	0.46
1:G:122:PHE:CE1	2:H:123:GLN:HG3	2.51	0.46
1:G:139:GLY:HA3	1:G:181:VAL:HG12	1.98	0.46
1:E:1:GLN:CD	1:E:1:GLN:N	2.74	0.46
2:D:121:ASP:HA	2:D:124:LEU:HD12	1.97	0.45
1:A:39:GLN:OE1	6:A:355:HOH:O	2.20	0.45
2:F:139:TYR:CG	2:F:140:PRO:HA	2.52	0.45
1:A:110:THR:HG22	6:A:245:HOH:O	2.12	0.45
1:G:182:VAL:HG22	1:G:183:THR:N	2.31	0.45
1:C:23:LYS:NZ	6:C:511:HOH:O	2.49	0.45
1:E:210:ARG:CD	1:E:210:ARG:C	2.88	0.45
2:B:189:LYS:HZ1	2:B:210:ARG:HG3	1.81	0.45
2:F:89:MET:HE2	2:F:97:PHE:CE2	2.51	0.45
1:A:197:ASN:HD22	1:A:207:VAL:HG13	1.82	0.45
1:G:100(C):ASN:OD1	1:G:100(D):HIS:N	2.50	0.44
2:H:93:GLU:HA	6:H:435:HOH:O	2.16	0.44
2:B:13:VAL:HG21	2:B:19:ALA:HB2	2.00	0.44
1:G:57:THR:HG21	1:G:69:LEU:HB2	1.99	0.44
2:H:131:VAL:HB	2:H:178:LEU:HD13	2.00	0.44
2:B:189:LYS:NZ	2:B:210:ARG:HG3	2.33	0.44
1:A:71:ARG:NH2	6:A:320:HOH:O	2.50	0.44
2:B:89:MET:HE2	2:B:97:PHE:CZ	2.52	0.44
2:B:124:LEU:HD23	2:B:124:LEU:HA	1.85	0.44
1:E:210:ARG:NH1	1:E:211:VAL:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82(C):LEU:HD13	1:G:111:VAL:CG2	2.47	0.44
1:A:209:LYS:O	1:A:210:ARG:NH1	2.51	0.44
2:D:14:THR:O	2:D:15:PRO:C	2.61	0.44
2:F:162:VAL:HG22	2:F:174:LEU:HD12	2.00	0.44
1:G:183:THR:O	1:G:184:VAL:HG23	2.18	0.44
2:D:40:PRO:HB3	2:D:164:GLU:HG3	2.00	0.43
1:E:126:PRO:HD3	1:E:138:LEU:HB3	1.99	0.43
2:H:13:VAL:HG21	2:H:19:ALA:HB2	2.00	0.43
1:C:100(H):LEU:N	1:C:100(H):LEU:HD23	2.32	0.43
1:E:201:LYS:H	1:E:201:LYS:HG3	1.66	0.43
2:B:133:CYS:HB2	2:B:147:TRP:CH2	2.54	0.43
1:E:13:LYS:O	1:E:14:PRO:C	2.59	0.43
2:H:135:LEU:HD11	2:H:195:VAL:HG21	2.01	0.43
1:E:135:THR:N	6:E:285:HOH:O	2.51	0.42
1:E:146:PHE:HB2	1:E:175:LEU:HD23	2.00	0.42
2:D:63:SER:O	2:D:73:LEU:HD12	2.18	0.42
2:H:27(D):HIS:HB3	2:H:28:ASN:OD1	2.18	0.42
2:D:174:LEU:C	2:D:174:LEU:HD23	2.44	0.42
2:B:197:HIS:CG	2:B:198:GLN:H	2.37	0.42
2:F:76:SER:O	2:F:77:ARG:C	2.61	0.42
1:G:6:GLN:NE2	1:G:107:THR:HG23	2.33	0.42
1:G:80:MET:HE3	1:G:80:MET:HB3	1.94	0.42
1:G:20:VAL:CG1	1:G:107:THR:HG21	2.50	0.42
2:H:33:LEU:HG	2:H:34:ASP:N	2.35	0.42
2:H:193:CYS:O	2:H:205:THR:HA	2.20	0.42
2:B:209:ASN:O	2:B:210:ARG:CB	2.67	0.42
2:F:187:LYS:HD2	2:F:188:HIS:CE1	2.54	0.42
1:A:29:PHE:CG	1:A:76:SER:CB	3.02	0.42
2:B:60:HIS:O	2:B:62:PHE:N	2.53	0.42
1:C:30:VAL:HB	6:C:240:HOH:O	2.20	0.42
2:H:93:GLU:O	2:H:94:SER:C	2.62	0.41
2:H:117:PHE:HD2	2:H:132:VAL:HG12	1.85	0.41
2:D:4:MET:CE	2:D:23:CYS:SG	3.08	0.41
2:D:7:SER:HA	2:D:8:PRO:C	2.45	0.41
1:E:143:LYS:HG2	1:E:144:ASP:CG	2.45	0.41
2:D:14:THR:HB	2:D:17:GLU:HG3	2.02	0.41
2:H:192:ALA:HB1	2:H:205:THR:HG22	2.02	0.41
1:A:195:ILE:HG21	1:A:207:VAL:HG12	2.02	0.41
2:D:179:THR:O	2:D:180:LEU:HD23	2.21	0.41
1:E:66:ARG:HH22	1:E:86:ASP:CG	2.25	0.41
1:C:197:ASN:HD22	1:C:207:VAL:HG22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:ALA:HB1	1:E:212:GLU:H	1.85	0.41
1:G:166:PHE:C	1:G:178:LEU:HD21	2.42	0.41
1:C:136:ALA:CB	1:C:186:SER:HB3	2.50	0.41
1:A:47:TRP:CZ3	1:A:49:GLY:HA2	2.56	0.41
2:B:139:TYR:CD2	2:B:140:PRO:HA	2.56	0.41
2:B:189:LYS:HZ1	2:B:210:ARG:CG	2.33	0.41
2:B:174:LEU:HD23	2:B:175:SER:N	2.35	0.41
2:B:189:LYS:O	2:B:209:ASN:HA	2.20	0.41
1:E:67:VAL:HG22	1:E:82:LEU:HD13	2.03	0.41
1:E:136:ALA:O	1:E:183:THR:HA	2.21	0.41
2:F:139:TYR:CD2	2:F:140:PRO:HA	2.56	0.41
1:G:82(C):LEU:HB3	1:G:111:VAL:HG11	2.03	0.41
1:G:167:PRO:O	1:G:178:LEU:HD23	2.21	0.41
2:H:116:ILE:HD12	2:H:193:CYS:HB2	2.02	0.41
2:D:93:GLU:O	2:D:94:SER:C	2.63	0.40
2:F:200:LEU:HD13	2:F:204:VAL:HG13	2.03	0.40
1:G:101:GLU:HG3	1:G:102:PHE:CD2	2.56	0.40
1:C:201:LYS:H	1:C:201:LYS:HG3	1.75	0.40
2:F:48:ILE:HA	2:F:53:ASN:O	2.22	0.40
1:A:13:LYS:O	1:A:14:PRO:C	2.64	0.40
1:G:20:VAL:HG13	1:G:107:THR:HG21	2.03	0.40
1:A:54:ARG:HB2	1:A:56:ASP:OD1	2.21	0.40
2:B:174:LEU:C	2:B:174:LEU:CD2	2.95	0.40
2:B:60:HIS:O	2:B:61:ARG:C	2.63	0.40
2:D:39:LYS:O	2:D:40:PRO:C	2.65	0.40
2:F:209:ASN:O	2:F:210:ARG:HB2	2.19	0.40

All (3) 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)
6:E:226:HOH:O	6:F:565:HOH:O[4_555]	1.41	0.79
6:E:558:HOH:O	6:F:384:HOH:O[4_555]	1.57	0.63
4:G:222:CL:CL	6:F:446:HOH:O[3_554]	1.75	0.45

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	212/232 (91%)	198 (93%)	13 (6%)	1 (0%)	24	46
1	C	207/232 (89%)	194 (94%)	11 (5%)	2 (1%)	12	28
1	E	208/232 (90%)	198 (95%)	9 (4%)	1 (0%)	24	46
1	G	176/232 (76%)	165 (94%)	10 (6%)	1 (1%)	21	42
2	B	213/218 (98%)	208 (98%)	4 (2%)	1 (0%)	24	46
2	D	213/218 (98%)	202 (95%)	11 (5%)	0	100	100
2	F	208/218 (95%)	201 (97%)	7 (3%)	0	100	100
2	H	175/218 (80%)	170 (97%)	5 (3%)	0	100	100
All	All	1612/1800 (90%)	1536 (95%)	70 (4%)	6 (0%)	30	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	185	PRO
2	B	61	ARG
1	C	156	SER
1	C	202	PRO
1	A	76	SER
1	G	149	PRO

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	186/200 (93%)	174 (94%)	12 (6%)	15	35
1	C	184/200 (92%)	168 (91%)	16 (9%)	9	21
1	E	185/200 (92%)	166 (90%)	19 (10%)	7	15
1	G	164/200 (82%)	151 (92%)	13 (8%)	11	26
2	B	189/191 (99%)	177 (94%)	12 (6%)	16	36
2	D	189/191 (99%)	177 (94%)	12 (6%)	16	36
2	F	186/191 (97%)	172 (92%)	14 (8%)	12	28
2	H	171/191 (90%)	152 (89%)	19 (11%)	6	12
All	All	1454/1564 (93%)	1337 (92%)	117 (8%)	11	25

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	30	VAL
1	A	66	ARG
1	A	71	ARG
1	A	110	THR
1	A	135	THR
1	A	178	LEU
1	A	184	VAL
1	A	203	SER
1	A	205	THR
1	A	210	ARG
1	A	211	VAL
2	B	10	SER
2	B	37	LEU
2	B	48	ILE
2	B	56	THR
2	B	89	MET
2	B	102	LYS
2	B	107	ARG
2	B	122	GLU
2	B	128	THR
2	B	178	LEU
2	B	196	THR
2	B	204	VAL
1	C	1	GLN
1	C	30	VAL
1	C	38	ARG

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Mol	Chain	Res	Type
1	C	43	GLN
1	C	54	ARG
1	C	64	LYS
1	C	68	THR
1	C	71	ARG
1	C	108	LEU
1	C	159	LEU
1	C	178	LEU
1	C	182	VAL
1	C	188	SER
1	C	192	GLN
1	C	210	ARG
1	C	211	VAL
2	D	1	ASP
2	D	17	GLU
2	D	37	LEU
2	D	92	LYS
2	D	102	LYS
2	D	107	ARG
2	D	121	ASP
2	D	142	GLU
2	D	155	SER
2	D	167	SER
2	D	184	ASP
2	D	206	LYS
1	E	30	VAL
1	E	38	ARG
1	E	89	ILE
1	E	107	THR
1	E	110	THR
1	E	135	THR
1	E	138	LEU
1	E	156	SER
1	E	160	THR
1	E	184	VAL
1	E	189	LEU
1	E	192	GLN
1	E	201	LYS
1	E	203	SER
1	E	204	ASN
1	E	205	THR
1	E	210	ARG

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Mol	Chain	Res	Type
1	E	211	VAL
1	E	212	GLU
2	F	11	LEU
2	F	33	LEU
2	F	37	LEU
2	F	47	LEU
2	F	77	ARG
2	F	102	LYS
2	F	107	ARG
2	F	126	SER
2	F	153	LEU
2	F	178	LEU
2	F	196	THR
2	F	204	VAL
2	F	205	THR
2	F	210	ARG
1	G	23	LYS
1	G	30	VAL
1	G	70	THR
1	G	107	THR
1	G	110	THR
1	G	115	SER
1	G	138	LEU
1	G	160	THR
1	G	172	SER
1	G	175	LEU
1	G	178	LEU
1	G	184	VAL
1	G	196	CYS
2	H	5	THR
2	H	37	LEU
2	H	42	GLN
2	H	47	LEU
2	H	89	MET
2	H	92	LYS
2	H	102	LYS
2	H	104	GLU
2	H	107	ARG
2	H	121	ASP
2	H	124	LEU
2	H	125	LYS
2	H	131	VAL

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Mol	Chain	Res	Type
2	H	142	GLU
2	H	155	SER
2	H	175	SER
2	H	178	LEU
2	H	193	CYS
2	H	205	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	192	GLN
2	B	38	GLN
2	B	159	GLN
2	B	209	ASN
1	C	39	GLN
2	D	38	GLN
2	D	42	GLN
2	D	136	ASN
2	D	137	ASN
2	D	188	HIS
1	E	3	GLN
1	E	43	GLN
2	F	123	GLN
2	F	137	ASN
1	G	164	HIS
1	G	199	ASN
2	H	137	ASN
2	H	154	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	H	214	-	5,5,5	0.65	0	5,5,5	0.27	0
5	GOL	D	214	-	5,5,5	0.32	0	5,5,5	0.69	0
3	SO4	A	221	-	4,4,4	0.27	0	6,6,6	0.74	0
3	SO4	E	221	-	4,4,4	0.27	0	6,6,6	0.48	0
3	SO4	G	221	-	4,4,4	0.18	0	6,6,6	0.22	0
5	GOL	F	214	-	5,5,5	0.49	0	5,5,5	1.10	0
5	GOL	E	222	-	5,5,5	0.63	0	5,5,5	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	GOL	E	222	-	-	2/4/4/4	-
5	GOL	F	214	-	-	0/4/4/4	-
5	GOL	D	214	-	-	2/4/4/4	-
5	GOL	H	214	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	214	GOL	C1-C2-C3-O3
5	E	222	GOL	O1-C1-C2-C3
5	H	214	GOL	O1-C1-C2-O2
5	H	214	GOL	O1-C1-C2-C3
5	D	214	GOL	O2-C2-C3-O3
5	E	222	GOL	O1-C1-C2-O2
5	H	214	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	221	SO4	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, 95th 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	216/232 (93%)	-0.44	4 (1%) 66 61	12, 29, 62, 72	0
1	C	213/232 (91%)	-0.34	3 (1%) 73 69	12, 30, 68, 78	0
1	E	214/232 (92%)	-0.23	5 (2%) 61 55	13, 37, 73, 89	0
1	G	192/232 (82%)	0.06	11 (5%) 29 24	14, 45, 81, 91	0
2	B	215/218 (98%)	-0.55	0 100 100	11, 32, 49, 59	0
2	D	215/218 (98%)	-0.55	0 100 100	12, 33, 57, 70	0
2	F	212/218 (97%)	-0.12	3 (1%) 73 69	15, 40, 84, 94	0
2	H	193/218 (88%)	0.14	7 (3%) 46 40	21, 48, 91, 103	0
All	All	1670/1800 (92%)	-0.26	33 (1%) 65 60	11, 35, 77, 103	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	183	ALA	5.6
1	C	210	ARG	4.1
1	G	125	ALA	3.4
1	E	210	ARG	3.4
2	H	140	PRO	3.4
1	E	189	LEU	3.3
1	E	211	VAL	3.3
2	H	178	LEU	3.2
1	A	211	VAL	3.0
2	H	148	LYS	2.9
1	G	199	ASN	2.7
1	C	188	SER	2.7
1	G	160	THR	2.7
1	C	202	PRO	2.6
1	G	1	GLN	2.5
2	F	192	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	193	THR	2.5
1	E	206	LYS	2.5
1	A	210	ARG	2.4
1	E	158	ALA	2.4
1	G	140	CYS	2.3
1	G	157	GLY	2.3
1	G	196	CYS	2.2
2	F	180	LEU	2.2
1	A	202	PRO	2.2
1	G	135	THR	2.1
2	H	142	GLU	2.1
2	H	124	LEU	2.1
2	F	151	ASN	2.1
1	G	169	VAL	2.0
2	H	205	THR	2.0
1	G	201	LYS	2.0
1	A	135	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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
4	CL	D	215	1/1	0.90	0.07	50,50,50,50	0
5	GOL	H	214	6/6	0.90	0.17	53,54,54,55	0
5	GOL	D	214	6/6	0.91	0.14	50,51,51,53	0
4	CL	B	216	1/1	0.91	0.06	50,50,50,50	0
5	GOL	F	214	6/6	0.92	0.12	38,41,48,51	0
4	CL	B	215	1/1	0.92	0.25	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	E	222	6/6	0.93	0.11	43,47,48,49	0
4	CL	B	214	1/1	0.94	0.09	51,51,51,51	0
3	SO4	A	221	5/5	0.94	0.10	55,55,56,59	0
4	CL	A	222	1/1	0.95	0.21	46,46,46,46	0
4	CL	F	215	1/1	0.95	0.17	63,63,63,63	0
4	CL	C	222	1/1	0.95	0.23	58,58,58,58	0
3	SO4	E	221	5/5	0.96	0.07	53,54,55,58	0
4	CL	H	215	1/1	0.96	0.13	59,59,59,59	0
3	SO4	G	221	5/5	0.96	0.07	63,63,64,65	0
4	CL	G	222	1/1	0.97	0.14	54,54,54,54	0
4	CL	C	221	1/1	0.98	0.18	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.