



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:09 AM UTC

PDB ID : 3O4L / pdb_00003o4l
Title : Genetic and structural basis for selection of a ubiquitous T cell receptor deployed in Epstein-Barr virus
Authors : Miles, J.J.; Bulek, A.M.; Cole, D.K.; Gostick, E.; Schauenburg, J.A.; Dolton, G.; Venturi, V.; Davenport, M.P.; Tan, M.P.; Burrows, S.R.; Wooldridge, L.; Price, D.A.; Rizkallah, P.J.; Sewell, A.K.
Deposited on : 2010-07-27
Resolution : 2.54 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

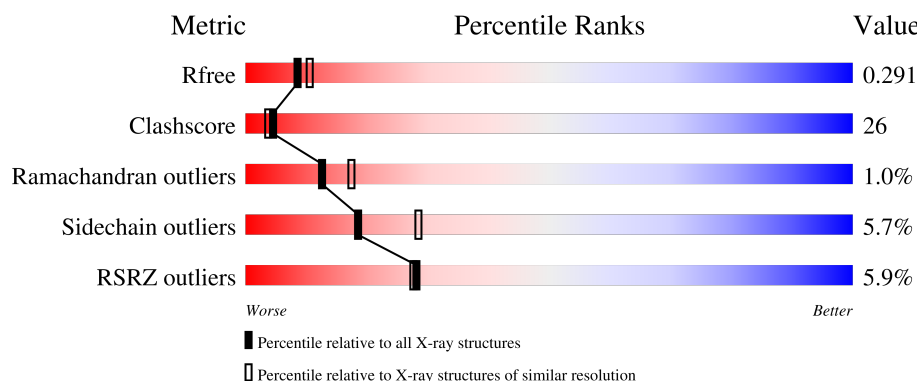
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	276	4% 74% 23% .
2	B	100	6% 57% 36% 7%
3	C	9	67% 33%
4	D	195	14% 53% 34% 10% .

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Mol	Chain	Length	Quality of chain
5	E	245	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	D	202	-	-	X	-
6	GOL	E	250	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7067 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			834	530	140	159	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P61769
B	91	CYS	LYS	engineered mutation	UNP P61769

- Molecule 3 is a protein called BSLF2/BMLF1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			62	40	9	11	2			

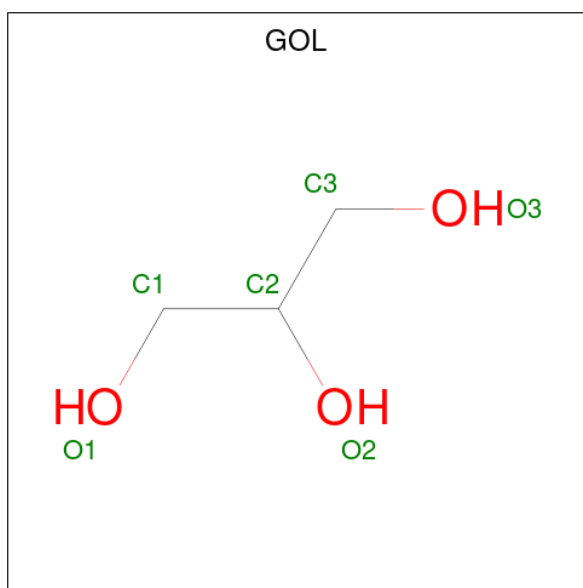
- Molecule 4 is a protein called T-CELL RECEPTOR, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	195	Total	C	N	O	S	0	0	0
			1538	960	254	314	10			

- Molecule 5 is a protein called T-CELL RECEPTOR, BETA CHAIN.

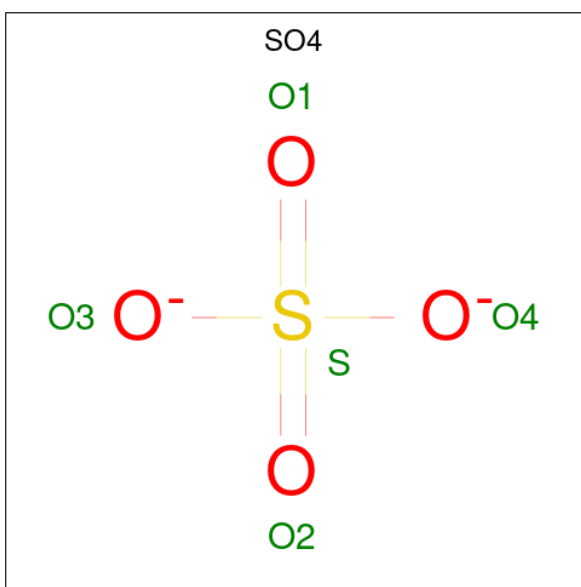
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1930	1215	331	375	9			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



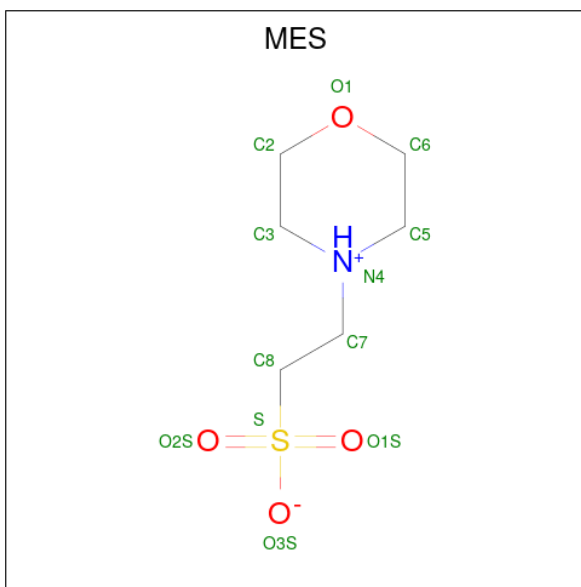
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

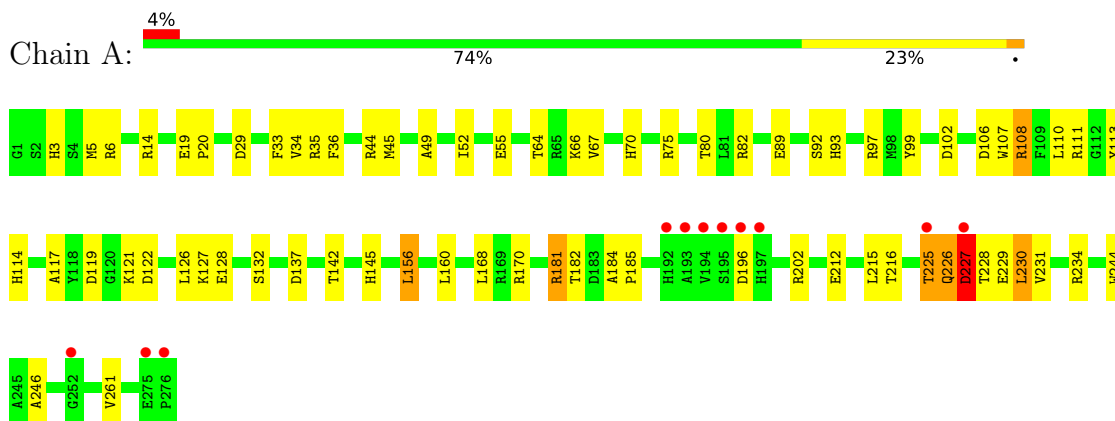
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	106	Total	O	0	0
			106	106		
9	B	48	Total	O	0	0
			48	48		
9	C	3	Total	O	0	0
			3	3		
9	D	76	Total	O	0	0
			76	76		
9	E	101	Total	O	0	2
			103	103		

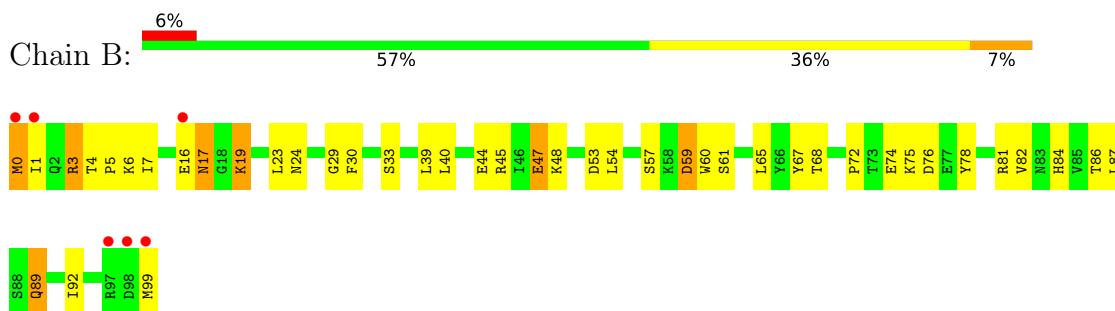
3 Residue-property plots

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.

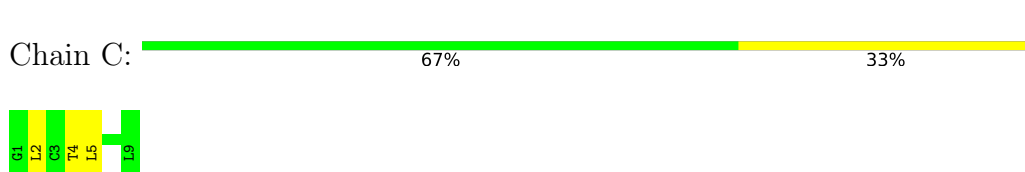
- Molecule 1: MHC class I antigen



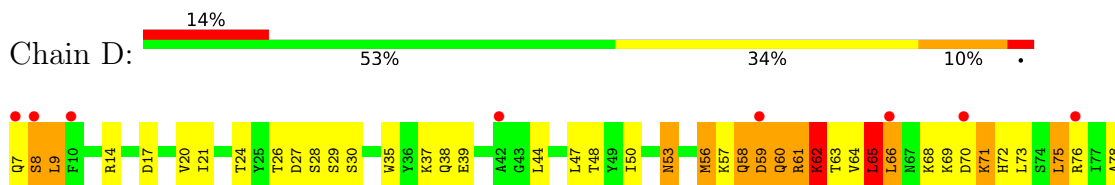
- Molecule 2: Beta-2-microglobulin

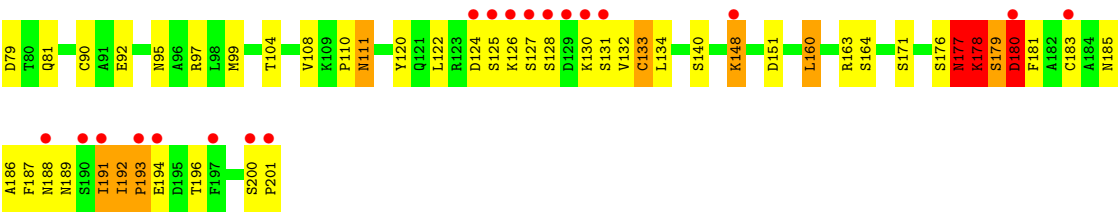


- Molecule 3: BSLF2/BMLF1 protein

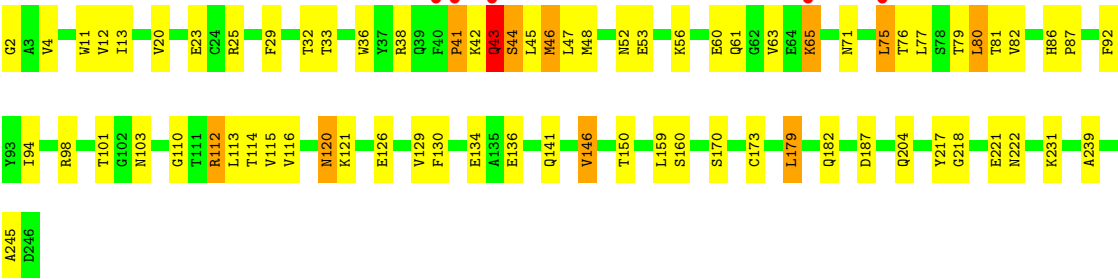


- Molecule 4: T-CELL RECEPTOR, ALPHA CHAIN





● Molecule 5: T-CELL RECEPTOR, BETA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.08Å 122.50Å 82.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.25 – 2.54 61.25 – 2.54	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.25-2.54) 99.0 (61.25-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.55Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.296 0.218 , 0.291	Depositor DCC
R_{free} test set	1603 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7067	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, GOL, MES

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	0.96	2/2320 (0.1%)	0.78	2/3149 (0.1%)
2	B	0.93	0/857	0.88	3/1159 (0.3%)
3	C	1.09	0/61	0.81	0/80
4	D	1.17	12/1568 (0.8%)	0.95	5/2123 (0.2%)
5	E	1.02	0/1981	0.90	6/2695 (0.2%)
All	All	1.03	14/6787 (0.2%)	0.87	16/9206 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	58	GLN	CA-C	-7.50	1.42	1.53
4	D	133	CYS	CB-SG	-7.16	1.57	1.81
4	D	62	LYS	N-CA	-7.15	1.36	1.46
4	D	194	GLU	CA-C	-6.78	1.43	1.52
4	D	183	CYS	CA-CB	-6.45	1.42	1.53
4	D	65	LEU	CA-C	-5.97	1.45	1.52
4	D	133	CYS	CA-CB	-5.85	1.42	1.53
1	A	225	THR	CA-C	-5.77	1.46	1.52
4	D	61	ARG	N-CA	-5.64	1.39	1.46
1	A	227	ASP	CA-C	-5.39	1.45	1.52
4	D	178	LYS	CA-C	-5.31	1.45	1.52
4	D	59	ASP	N-CA	-5.27	1.39	1.46
4	D	192	ILE	N-CA	-5.20	1.42	1.46
4	D	183	CYS	CA-C	-5.03	1.45	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	179	SER	N-CA-C	11.37	125.42	112.57
5	E	44	SER	N-CA-C	11.25	125.95	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	59	ASP	N-CA-C	-10.07	97.24	110.53
4	D	180	ASP	N-CA-C	-9.51	101.87	113.19
5	E	43	GLN	N-CA-C	7.93	127.68	110.80
4	D	178	LYS	N-CA-C	-6.91	96.09	110.80
2	B	47	GLU	N-CA-C	6.73	121.49	113.28
5	E	222	ASN	N-CA-C	-6.26	104.56	111.82
1	A	225	THR	N-CA-C	-5.94	105.03	112.93
5	E	126	GLU	N-CA-C	-5.68	101.02	110.17
4	D	183	CYS	CA-CB-SG	-5.67	101.35	114.40
1	A	137	ASP	N-CA-C	5.46	115.33	108.45
5	E	182	GLN	CA-C-N	5.10	124.55	119.24
5	E	182	GLN	C-N-CA	5.10	124.55	119.24
4	D	177	ASN	N-CA-C	-5.09	100.60	108.90
2	B	17	ASN	N-CA-C	5.01	117.37	110.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2254	0	2103	74	0
2	B	834	0	795	52	1
3	C	62	0	73	2	0
4	D	1538	0	1466	143	0
5	E	1930	0	1837	103	1
6	A	18	0	24	5	0
6	B	6	0	8	1	0
6	D	12	0	16	7	0
6	E	30	0	40	10	0
7	A	10	0	0	0	0
7	B	10	0	0	1	0
7	E	15	0	0	0	0
8	B	12	0	12	0	0
9	A	106	0	0	5	0
9	B	48	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	3	0	0	0	0
9	D	76	0	0	2	0
9	E	103	0	0	2	0
All	All	7067	0	6374	343	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 26.

All (343) 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:D:7:GLN:O	5:E:43:GLN:HG2	1.31	1.29
4:D:26:THR:HG22	4:D:92:GLU:OE2	1.36	1.24
4:D:192:ILE:CD1	4:D:196:THR:HG21	1.68	1.22
4:D:61:ARG:HG3	4:D:62:LYS:HG3	1.32	1.12
4:D:61:ARG:HG3	4:D:62:LYS:H	1.12	1.11
4:D:61:ARG:CG	4:D:62:LYS:H	1.60	1.09
4:D:192:ILE:HD13	4:D:196:THR:HG21	1.20	1.07
5:E:112:ARG:HG2	5:E:112:ARG:HH21	1.15	1.06
2:B:0:MET:N	2:B:0:MET:HE3	1.71	1.04
4:D:7:GLN:HG2	4:D:8:SER:H	1.22	1.02
5:E:43:GLN:O	5:E:44:SER:HB2	1.60	0.99
4:D:58:GLN:HG2	4:D:58:GLN:O	1.60	0.98
4:D:7:GLN:O	5:E:43:GLN:CG	2.11	0.97
4:D:177:ASN:O	4:D:178:LYS:HB3	1.64	0.94
4:D:178:LYS:O	4:D:178:LYS:HG2	1.68	0.91
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.36	0.90
4:D:60:GLN:HG3	4:D:61:ARG:N	1.83	0.89
2:B:0:MET:HE3	2:B:0:MET:H2	1.37	0.89
1:A:226:GLN:O	1:A:227:ASP:HB2	1.73	0.88
5:E:101:THR:HG22	9:E:343:HOH:O	1.72	0.87
4:D:192:ILE:CD1	4:D:196:THR:CG2	2.52	0.87
4:D:76:ARG:NH2	4:D:78:ALA:HB2	1.90	0.87
2:B:29:GLY:HA2	2:B:61:SER:OG	1.75	0.86
4:D:60:GLN:CG	4:D:61:ARG:N	2.39	0.86
5:E:43:GLN:N	5:E:43:GLN:HE21	1.74	0.85
4:D:66:LEU:HD12	4:D:66:LEU:O	1.74	0.85
1:A:114:HIS:CD2	1:A:156:LEU:HD11	2.11	0.85
4:D:177:ASN:H	4:D:177:ASN:HD22	1.25	0.85
1:A:49:ALA:O	1:A:52:ILE:HG22	1.77	0.84
5:E:112:ARG:HH21	5:E:112:ARG:CG	1.89	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:THR:OG1	2:B:86:THR:HG21	1.78	0.84
4:D:57:LYS:O	4:D:65:LEU:HD13	1.78	0.84
5:E:112:ARG:HG2	5:E:112:ARG:NH2	1.91	0.84
4:D:132:VAL:HG21	5:E:146:VAL:HG21	1.59	0.84
1:A:226:GLN:O	1:A:226:GLN:HG2	1.75	0.84
4:D:61:ARG:HG3	4:D:62:LYS:CG	2.09	0.83
1:A:230:LEU:C	1:A:230:LEU:CD2	2.51	0.83
4:D:61:ARG:CG	4:D:62:LYS:N	2.36	0.83
4:D:61:ARG:HG3	4:D:62:LYS:N	1.91	0.82
4:D:61:ARG:CG	4:D:62:LYS:HG3	2.08	0.82
5:E:71:ASN:OD1	5:E:79:THR:HB	1.79	0.82
4:D:124:ASP:CG	4:D:126:LYS:O	2.24	0.81
4:D:131:SER:HG	6:D:6:GOL:HO2	1.19	0.81
1:A:108:ARG:HH11	1:A:108:ARG:CG	1.94	0.81
1:A:230:LEU:HD21	9:A:296:HOH:O	1.80	0.80
5:E:159:LEU:HD23	5:E:160:SER:N	1.96	0.80
1:A:97:ARG:HE	1:A:114:HIS:HE1	1.30	0.79
4:D:37:LYS:NZ	4:D:39:GLU:OE2	2.16	0.78
4:D:68:LYS:O	4:D:70:ASP:N	2.17	0.77
1:A:230:LEU:O	1:A:230:LEU:HD22	1.85	0.77
5:E:56:LYS:H	5:E:56:LYS:HD2	1.49	0.77
5:E:129:VAL:HG23	5:E:239:ALA:HB3	1.67	0.77
4:D:7:GLN:HG2	4:D:8:SER:N	1.99	0.77
4:D:26:THR:CG2	4:D:92:GLU:OE2	2.28	0.76
4:D:160:LEU:HD12	4:D:160:LEU:O	1.87	0.75
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.20	0.75
4:D:65:LEU:HD13	4:D:65:LEU:N	2.01	0.75
4:D:148:LYS:HB2	4:D:148:LYS:NZ	2.01	0.75
4:D:7:GLN:HA	5:E:43:GLN:HB2	1.68	0.75
5:E:221:GLU:HA	5:E:231:LYS:HZ1	1.50	0.74
5:E:130:PHE:HB2	5:E:146:VAL:HG22	1.71	0.73
5:E:38:ARG:HG3	5:E:48:MET:SD	2.29	0.72
5:E:45:LEU:HD21	5:E:94:ILE:HD12	1.71	0.72
4:D:95:ASN:N	6:D:202:GOL:O2	2.17	0.72
4:D:65:LEU:N	4:D:65:LEU:CD1	2.53	0.72
5:E:25:ARG:HG3	5:E:76:THR:HG22	1.71	0.71
4:D:191:ILE:HD13	4:D:191:ILE:C	2.15	0.71
4:D:177:ASN:O	4:D:177:ASN:ND2	2.22	0.71
1:A:230:LEU:C	1:A:230:LEU:HD22	2.15	0.71
4:D:160:LEU:HD12	4:D:160:LEU:C	2.16	0.70
4:D:97:ARG:HD2	5:E:47:LEU:CD2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:66:LEU:HD12	4:D:66:LEU:C	2.16	0.70
4:D:68:LYS:C	4:D:70:ASP:H	2.00	0.69
5:E:43:GLN:N	5:E:43:GLN:NE2	2.40	0.69
4:D:7:GLN:CA	5:E:43:GLN:HB2	2.23	0.69
5:E:42:LYS:HB3	5:E:43:GLN:NE2	2.08	0.68
5:E:43:GLN:O	5:E:44:SER:CB	2.33	0.68
1:A:215:LEU:O	1:A:216:THR:HG23	1.94	0.68
5:E:179:LEU:C	5:E:179:LEU:HD12	2.18	0.68
4:D:192:ILE:HD11	4:D:196:THR:HG21	1.74	0.67
4:D:65:LEU:HD13	4:D:65:LEU:H	1.61	0.66
5:E:12:VAL:HG13	5:E:113:LEU:CD1	2.25	0.66
4:D:7:GLN:CG	4:D:8:SER:H	1.94	0.66
1:A:229:GLU:HG3	1:A:229:GLU:O	1.96	0.66
5:E:221:GLU:HA	5:E:231:LYS:NZ	2.11	0.65
4:D:30:SER:HA	6:D:202:GOL:H2	1.79	0.65
2:B:0:MET:HE3	2:B:0:MET:CA	2.26	0.64
5:E:60:GLU:O	5:E:63:VAL:HG22	1.98	0.64
1:A:82:ARG:HD2	1:A:89:GLU:HA	1.80	0.64
5:E:56:LYS:HD2	5:E:56:LYS:N	2.12	0.64
5:E:46:MET:HE2	5:E:46:MET:HA	1.78	0.64
2:B:84:HIS:HB3	2:B:87:LEU:HD23	1.80	0.63
2:B:47:GLU:O	2:B:48:LYS:HG3	1.98	0.63
5:E:20:VAL:CG1	5:E:82:VAL:HB	2.29	0.62
2:B:24:ASN:HD22	2:B:67:TYR:HB3	1.65	0.62
4:D:60:GLN:HG3	4:D:61:ARG:H	1.62	0.62
4:D:177:ASN:HD22	4:D:177:ASN:N	1.96	0.62
4:D:21:ILE:N	4:D:21:ILE:HD12	2.15	0.62
4:D:192:ILE:HD13	4:D:196:THR:CG2	2.13	0.62
5:E:33:THR:OG1	5:E:52:ASN:ND2	2.33	0.61
4:D:97:ARG:HD2	5:E:47:LEU:HD23	1.82	0.61
4:D:179:SER:C	4:D:181:PHE:H	2.07	0.61
1:A:35:ARG:HG2	1:A:36:PHE:N	2.13	0.61
5:E:204:GLN:O	5:E:245:ALA:HB2	2.01	0.60
4:D:124:ASP:OD2	4:D:128:SER:HB2	2.01	0.60
4:D:66:LEU:C	4:D:66:LEU:CD1	2.75	0.60
4:D:122:LEU:CD2	5:E:146:VAL:HG13	2.31	0.60
4:D:180:ASP:OD2	4:D:180:ASP:C	2.43	0.60
4:D:200:SER:HB2	4:D:201:PRO:HD2	1.82	0.60
5:E:179:LEU:HD12	5:E:179:LEU:O	2.02	0.60
4:D:47:LEU:O	4:D:48:THR:HG23	2.02	0.60
5:E:159:LEU:HD23	5:E:159:LEU:C	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:218:GLY:O	6:E:250:GOL:H2	2.02	0.60
5:E:116:VAL:HB	5:E:121:LYS:HD3	1.83	0.59
4:D:64:VAL:HB	4:D:76:ARG:HB3	1.84	0.59
4:D:47:LEU:HD23	4:D:47:LEU:H	1.68	0.59
5:E:12:VAL:HG13	5:E:113:LEU:HD13	1.84	0.59
1:A:226:GLN:HG3	1:A:227:ASP:OD2	2.03	0.59
4:D:61:ARG:HG2	4:D:62:LYS:H	1.60	0.59
1:A:3:HIS:ND1	1:A:29:ASP:OD2	2.28	0.58
5:E:29:PHE:HA	6:E:249:GOL:H2	1.85	0.58
2:B:0:MET:HE3	2:B:0:MET:H1	1.66	0.58
1:A:230:LEU:C	1:A:230:LEU:HD23	2.26	0.58
1:A:19:GLU:HG3	1:A:20:PRO:HD2	1.86	0.58
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.39	0.58
5:E:75:LEU:N	5:E:75:LEU:HD12	2.19	0.57
5:E:43:GLN:NE2	5:E:43:GLN:CA	2.66	0.57
4:D:148:LYS:HB2	4:D:148:LYS:HZ3	1.67	0.57
2:B:0:MET:N	2:B:0:MET:CE	2.58	0.57
1:A:114:HIS:HD2	1:A:156:LEU:HD11	1.69	0.57
5:E:61:GLN:C	5:E:61:GLN:NE2	2.63	0.57
4:D:179:SER:C	4:D:181:PHE:N	2.62	0.56
5:E:103:ASN:HA	6:E:247:GOL:O2	2.06	0.56
4:D:58:GLN:O	4:D:58:GLN:CG	2.33	0.56
4:D:127:SER:OG	6:D:6:GOL:O1	2.21	0.56
4:D:79:ASP:OD1	4:D:79:ASP:O	2.23	0.56
1:A:35:ARG:HG3	2:B:53:ASP:OD2	2.06	0.56
1:A:66:LYS:O	1:A:70:HIS:HD2	1.89	0.55
4:D:7:GLN:C	5:E:43:GLN:HB2	2.30	0.55
1:A:75:ARG:NH2	5:E:53:GLU:O	2.39	0.55
4:D:7:GLN:CG	4:D:8:SER:N	2.61	0.55
5:E:25:ARG:HG3	5:E:76:THR:CG2	2.37	0.55
5:E:20:VAL:HG12	5:E:82:VAL:HB	1.89	0.55
4:D:124:ASP:C	4:D:126:LYS:H	2.14	0.55
5:E:23:GLU:HB3	5:E:77:LEU:HD11	1.89	0.55
5:E:80:LEU:HD23	5:E:81:THR:N	2.22	0.55
4:D:47:LEU:O	4:D:48:THR:CG2	2.55	0.55
2:B:6:LYS:HB2	2:B:6:LYS:NZ	2.22	0.54
1:A:215:LEU:O	1:A:216:THR:CG2	2.55	0.54
4:D:111:ASN:N	4:D:111:ASN:HD22	2.05	0.54
5:E:2:GLY:O	5:E:4:VAL:HG23	2.06	0.54
5:E:12:VAL:CG1	5:E:113:LEU:HD13	2.37	0.54
5:E:44:SER:OG	5:E:45:LEU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HD22	1:A:160:LEU:HG	1.87	0.54
2:B:57:SER:O	2:B:59:ASP:O	2.26	0.54
5:E:45:LEU:CD2	5:E:94:ILE:HD12	2.36	0.54
4:D:111:ASN:HD22	4:D:111:ASN:H	1.56	0.54
5:E:12:VAL:HG13	5:E:113:LEU:HD12	1.89	0.54
1:A:127:LYS:HD3	1:A:132:SER:HB3	1.90	0.53
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.88	0.53
5:E:12:VAL:HA	6:E:250:GOL:H11	1.90	0.53
1:A:114:HIS:CD2	1:A:156:LEU:CD1	2.88	0.53
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.76	0.53
2:B:89:GLN:NE2	9:B:122:HOH:O	2.40	0.53
5:E:112:ARG:CG	5:E:112:ARG:NH2	2.58	0.53
4:D:7:GLN:O	5:E:43:GLN:CB	2.56	0.53
4:D:59:ASP:O	4:D:59:ASP:OD2	2.27	0.53
4:D:47:LEU:HD23	4:D:47:LEU:N	2.24	0.53
4:D:192:ILE:HD12	4:D:193:PRO:O	2.09	0.53
4:D:130:LYS:HZ2	5:E:150:THR:HG21	1.75	0.52
1:A:106:ASP:O	1:A:107:TRP:HB2	2.09	0.52
5:E:217:TYR:HB3	6:E:250:GOL:H31	1.90	0.52
4:D:68:LYS:HB3	4:D:72:HIS:HB3	1.91	0.52
2:B:1:ILE:N	2:B:1:ILE:HD12	2.24	0.52
4:D:134:LEU:HD11	4:D:171:SER:HB2	1.92	0.52
1:A:119:ASP:O	2:B:1:ILE:HD13	2.09	0.52
4:D:124:ASP:C	4:D:126:LYS:N	2.67	0.52
1:A:14:ARG:NH1	9:A:357:HOH:O	2.38	0.52
4:D:120:TYR:CE1	5:E:136:GLU:HA	2.46	0.51
1:A:114:HIS:HD2	1:A:156:LEU:CD1	2.23	0.51
4:D:35:TRP:O	4:D:47:LEU:HD23	2.10	0.51
4:D:73:LEU:HD23	4:D:90:CYS:HB2	1.92	0.51
4:D:131:SER:OG	6:D:6:GOL:O2	2.01	0.51
4:D:63:THR:HG23	4:D:75:LEU:HD21	1.91	0.51
4:D:68:LYS:C	4:D:70:ASP:N	2.65	0.51
2:B:16:GLU:HB3	2:B:19:LYS:HG2	1.92	0.51
4:D:9:LEU:HD12	4:D:104:THR:HG23	1.93	0.51
4:D:160:LEU:C	4:D:160:LEU:CD1	2.83	0.50
1:A:97:ARG:HE	1:A:114:HIS:CE1	2.18	0.50
1:A:181:ARG:HG2	1:A:182:THR:N	2.25	0.50
4:D:122:LEU:HD12	4:D:122:LEU:N	2.27	0.50
2:B:24:ASN:ND2	2:B:67:TYR:HB3	2.26	0.50
2:B:29:GLY:CA	2:B:61:SER:OG	2.55	0.50
5:E:56:LYS:H	5:E:56:LYS:CD	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:HA	1:A:246:ALA:O	2.11	0.50
4:D:177:ASN:O	4:D:178:LYS:CB	2.43	0.50
1:A:225:THR:OG1	1:A:226:GLN:N	2.43	0.49
5:E:43:GLN:HE21	5:E:43:GLN:CA	2.25	0.49
2:B:4:THR:HG22	2:B:5:PRO:HD2	1.93	0.49
2:B:24:ASN:HD22	2:B:67:TYR:CB	2.25	0.49
1:A:244:TRP:NE1	2:B:99:MET:HG3	2.28	0.49
4:D:130:LYS:NZ	5:E:150:THR:HG21	2.28	0.49
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.47	0.49
4:D:95:ASN:H	6:D:202:GOL:HO2	1.51	0.49
1:A:111:ARG:NH1	1:A:128:GLU:HG3	2.28	0.49
4:D:111:ASN:H	4:D:111:ASN:ND2	2.10	0.49
4:D:132:VAL:C	4:D:133:CYS:SG	2.95	0.49
2:B:4:THR:CG2	2:B:5:PRO:HD2	2.43	0.49
4:D:185:ASN:OD1	4:D:185:ASN:C	2.55	0.49
1:A:226:GLN:O	1:A:227:ASP:CB	2.48	0.48
2:B:39:LEU:CD1	2:B:68:THR:HG22	2.44	0.48
4:D:20:VAL:C	4:D:21:ILE:HD12	2.38	0.48
5:E:65:LYS:HD3	5:E:65:LYS:O	2.12	0.48
5:E:179:LEU:C	5:E:179:LEU:CD1	2.86	0.48
2:B:76:ASP:HB3	2:B:78:TYR:CE2	2.48	0.48
1:A:97:ARG:NE	1:A:114:HIS:HE1	2.06	0.48
4:D:191:ILE:C	4:D:191:ILE:CD1	2.85	0.48
5:E:42:LYS:HB3	5:E:43:GLN:HE21	1.79	0.48
1:A:145:HIS:HB2	6:A:279:GOL:H32	1.96	0.48
4:D:47:LEU:C	4:D:48:THR:HG23	2.39	0.48
5:E:120:ASN:C	5:E:120:ASN:HD22	2.21	0.48
4:D:124:ASP:O	4:D:126:LYS:N	2.47	0.48
1:A:145:HIS:CB	6:A:279:GOL:H32	2.44	0.47
1:A:230:LEU:CD2	9:A:296:HOH:O	2.51	0.47
2:B:40:LEU:HA	2:B:44:GLU:O	2.14	0.47
5:E:36:TRP:HB3	5:E:48:MET:HE3	1.96	0.47
1:A:108:ARG:CG	1:A:108:ARG:NH1	2.63	0.47
2:B:87:LEU:N	2:B:87:LEU:HD22	2.29	0.47
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.49	0.47
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.96	0.47
4:D:151:ASP:OD1	4:D:151:ASP:N	2.46	0.47
4:D:148:LYS:HB2	4:D:148:LYS:HZ2	1.77	0.47
4:D:187:PHE:C	4:D:189:ASN:H	2.21	0.47
4:D:97:ARG:CZ	4:D:99:MET:HE3	2.45	0.47
1:A:126:LEU:HD22	1:A:156:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HE3	6:A:278:GOL:H11	1.97	0.46
1:A:142:THR:HG23	6:A:279:GOL:H12	1.97	0.46
2:B:74:GLU:OE1	2:B:74:GLU:C	2.59	0.46
4:D:38:GLN:HB2	4:D:44:LEU:HD23	1.97	0.46
4:D:44:LEU:HD11	5:E:45:LEU:HD11	1.97	0.46
1:A:55:GLU:OE2	1:A:170:ARG:NH1	2.47	0.46
4:D:97:ARG:CD	5:E:47:LEU:CD2	2.94	0.46
5:E:86:HIS:HB3	5:E:87:PRO:CD	2.46	0.46
1:A:75:ARG:NH1	5:E:53:GLU:OE1	2.49	0.46
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.97	0.46
1:A:231:VAL:CG1	1:A:244:TRP:CZ2	2.99	0.46
2:B:57:SER:C	2:B:59:ASP:O	2.59	0.46
4:D:122:LEU:HD22	5:E:146:VAL:HG13	1.97	0.46
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.97	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.51	0.45
4:D:185:ASN:OD1	4:D:186:ALA:N	2.50	0.45
4:D:185:ASN:O	4:D:188:ASN:HB3	2.16	0.45
1:A:111:ARG:HH12	1:A:128:GLU:CG	2.28	0.45
1:A:234:ARG:HH12	2:B:99:MET:HE2	1.80	0.45
4:D:24:THR:HA	4:D:71:LYS:O	2.16	0.45
1:A:215:LEU:C	1:A:216:THR:HG23	2.42	0.45
4:D:37:LYS:HB2	4:D:47:LEU:HD22	1.99	0.45
4:D:56:MET:HA	4:D:65:LEU:O	2.17	0.45
4:D:163:ARG:HG2	5:E:170:SER:OG	2.16	0.45
1:A:127:LYS:HB3	6:A:278:GOL:C1	2.47	0.45
5:E:86:HIS:HB3	5:E:87:PRO:HD2	1.98	0.45
4:D:27:ASP:OD2	4:D:27:ASP:C	2.59	0.45
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.52	0.44
4:D:176:SER:OG	4:D:178:LYS:HD3	2.17	0.44
4:D:110:PRO:O	4:D:140:SER:OG	2.33	0.44
5:E:25:ARG:HA	5:E:76:THR:O	2.17	0.44
1:A:93:HIS:HD2	1:A:119:ASP:OD1	2.01	0.44
2:B:4:THR:CB	2:B:86:THR:HG21	2.48	0.44
2:B:0:MET:H1	2:B:0:MET:CE	2.28	0.44
2:B:23:LEU:O	2:B:67:TYR:HA	2.18	0.44
4:D:14:ARG:HB2	4:D:17:ASP:OD1	2.18	0.44
1:A:82:ARG:NH1	9:A:300:HOH:O	2.50	0.43
5:E:11:TRP:C	6:E:250:GOL:H32	2.43	0.43
5:E:92:PHE:CZ	5:E:110:GLY:HA3	2.53	0.43
1:A:122:ASP:OD1	2:B:60:TRP:NE1	2.43	0.43
2:B:5:PRO:HD2	2:B:87:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:LEU:HD12	2:B:68:THR:HG22	2.00	0.43
4:D:97:ARG:HD2	5:E:47:LEU:HD21	1.98	0.43
4:D:177:ASN:O	4:D:177:ASN:CG	2.62	0.43
5:E:120:ASN:HD22	5:E:121:LYS:N	2.16	0.43
4:D:50:ILE:HD12	4:D:65:LEU:HD22	2.00	0.43
4:D:97:ARG:CD	5:E:47:LEU:HD21	2.49	0.43
4:D:192:ILE:HD12	4:D:192:ILE:C	2.43	0.43
5:E:221:GLU:HB3	9:E:259:HOH:O	2.18	0.43
2:B:81:ARG:HG3	2:B:92:ILE:CD1	2.49	0.43
2:B:17:ASN:HA	2:B:72:PRO:O	2.17	0.43
4:D:187:PHE:C	4:D:189:ASN:N	2.77	0.43
2:B:84:HIS:CD2	2:B:86:THR:H	2.36	0.43
2:B:59:ASP:OD1	2:B:59:ASP:C	2.62	0.43
4:D:9:LEU:HA	4:D:9:LEU:HD22	1.69	0.43
5:E:75:LEU:HD12	5:E:75:LEU:H	1.83	0.43
1:A:45:MET:HE1	3:C:2:LEU:HD11	2.01	0.43
5:E:121:LYS:NZ	5:E:187:ASP:OD1	2.45	0.42
2:B:40:LEU:N	2:B:40:LEU:CD1	2.82	0.42
5:E:45:LEU:O	5:E:46:MET:HE3	2.19	0.42
4:D:71:LYS:HD3	4:D:71:LYS:N	2.34	0.42
4:D:111:ASN:ND2	4:D:111:ASN:O	2.52	0.42
4:D:53:ASN:C	4:D:53:ASN:HD22	2.26	0.42
5:E:75:LEU:N	5:E:75:LEU:CD1	2.82	0.42
7:B:102:SO4:O1	9:B:169:HOH:O	2.21	0.42
4:D:163:ARG:O	4:D:164:SER:C	2.62	0.42
5:E:13:ILE:H	6:E:250:GOL:H11	1.83	0.42
1:A:196:ASP:OD1	1:A:196:ASP:O	2.38	0.42
1:A:212:GLU:OE2	1:A:212:GLU:HA	2.20	0.42
4:D:81:GLN:O	4:D:108:VAL:HG21	2.20	0.42
4:D:60:GLN:HG2	4:D:61:ARG:CB	2.50	0.42
5:E:134:GLU:CD	5:E:134:GLU:H	2.28	0.42
5:E:141:GLN:NE2	5:E:141:GLN:HA	2.34	0.42
5:E:98:ARG:NH2	6:E:247:GOL:O1	2.53	0.42
5:E:114:THR:HG23	6:E:1:GOL:O2	2.20	0.42
4:D:160:LEU:HB3	5:E:173:CYS:HB2	2.01	0.41
4:D:196:THR:HG23	9:D:235:HOH:O	2.20	0.41
2:B:6:LYS:HB2	2:B:6:LYS:HZ2	1.85	0.41
5:E:80:LEU:C	5:E:80:LEU:CD2	2.93	0.41
1:A:6:ARG:HH22	1:A:113:TYR:HE1	1.64	0.41
2:B:7:ILE:HD13	2:B:82:VAL:HG21	2.03	0.41
4:D:29:SER:HB3	6:D:202:GOL:H12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:SER:N	9:A:284:HOH:O	2.53	0.41
1:A:99:TYR:HB3	1:A:114:HIS:ND1	2.36	0.41
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.51	0.41
2:B:59:ASP:OD1	2:B:61:SER:HB3	2.20	0.41
5:E:80:LEU:HD23	5:E:80:LEU:C	2.45	0.41
5:E:221:GLU:HG2	5:E:231:LYS:HZ3	1.85	0.41
4:D:78:ALA:O	4:D:79:ASP:C	2.63	0.41
4:D:27:ASP:OD2	4:D:28:SER:N	2.54	0.41
4:D:124:ASP:CB	4:D:126:LYS:O	2.69	0.41
5:E:20:VAL:HG13	5:E:82:VAL:HB	2.02	0.41
5:E:87:PRO:HA	5:E:115:VAL:HB	2.01	0.41
1:A:184:ALA:HA	1:A:185:PRO:HD3	1.91	0.41
2:B:3:ARG:HB3	6:B:101:GOL:H31	2.03	0.41
4:D:62:LYS:HB3	4:D:78:ALA:HB3	2.03	0.41
4:D:79:ASP:OD1	4:D:79:ASP:C	2.63	0.41
4:D:97:ARG:HG3	5:E:47:LEU:HD21	2.03	0.41
4:D:111:ASN:N	4:D:111:ASN:ND2	2.68	0.41
1:A:64:THR:O	1:A:67:VAL:HG12	2.20	0.40
1:A:108:ARG:HG2	1:A:108:ARG:NH1	2.16	0.40
2:B:24:ASN:ND2	2:B:67:TYR:CB	2.85	0.40
3:C:4:THR:O	6:E:247:GOL:H11	2.21	0.40
4:D:7:GLN:O	5:E:43:GLN:HB2	2.20	0.40
4:D:164:SER:HB3	9:D:207:HOH:O	2.21	0.40
2:B:0:MET:CA	2:B:0:MET:CE	2.98	0.40
5:E:63:VAL:O	5:E:63:VAL:HG23	2.21	0.40
5:E:75:LEU:H	5:E:75:LEU:CD1	2.34	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)
2:B:45:ARG:NH2	5:E:221:GLU:OE2[2_565]	1.88	0.32

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	274/276 (99%)	264 (96%)	9 (3%)	1 (0%)	30	39
2	B	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	193/195 (99%)	170 (88%)	17 (9%)	6 (3%)	3	2
5	E	243/245 (99%)	228 (94%)	14 (6%)	1 (0%)	30	39
All	All	815/825 (99%)	760 (93%)	47 (6%)	8 (1%)	12	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	60	GLN
4	D	69	LYS
4	D	178	LYS
1	A	227	ASP
4	D	193	PRO
4	D	8	SER
4	D	125	SER
5	E	41	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	232/232 (100%)	223 (96%)	9 (4%)	28	43
2	B	95/95 (100%)	90 (95%)	5 (5%)	20	31
3	C	7/7 (100%)	6 (86%)	1 (14%)	3	3
4	D	178/178 (100%)	163 (92%)	15 (8%)	10	14
5	E	213/213 (100%)	202 (95%)	11 (5%)	21	32
All	All	725/725 (100%)	684 (94%)	41 (6%)	18	28

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	80	THR
1	A	108	ARG
1	A	110	LEU
1	A	121	LYS
1	A	156	LEU
1	A	181	ARG
1	A	226	GLN
1	A	230	LEU
2	B	0	MET
2	B	3	ARG
2	B	19	LYS
2	B	75	LYS
2	B	89	GLN
3	C	5	LEU
4	D	9	LEU
4	D	53	ASN
4	D	56	MET
4	D	62	LYS
4	D	65	LEU
4	D	66	LEU
4	D	71	LYS
4	D	75	LEU
4	D	111	ASN
4	D	148	LYS
4	D	160	LEU
4	D	177	ASN
4	D	178	LYS
4	D	180	ASP
4	D	191	ILE
5	E	32	THR
5	E	41	PRO
5	E	43	GLN
5	E	46	MET
5	E	65	LYS
5	E	75	LEU
5	E	80	LEU
5	E	112	ARG
5	E	120	ASN
5	E	146	VAL
5	E	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	72	GLN
1	A	93	HIS
1	A	114	HIS
1	A	115	GLN
1	A	174	ASN
1	A	188	HIS
1	A	191	HIS
1	A	224	GLN
1	A	242	GLN
1	A	253	GLN
1	A	255	GLN
1	A	262	GLN
2	B	24	ASN
2	B	51	HIS
2	B	84	HIS
4	D	22	ASN
4	D	38	GLN
4	D	53	ASN
4	D	111	ASN
4	D	114	ASN
4	D	143	ASN
4	D	146	GLN
4	D	177	ASN
4	D	189	ASN
5	E	39	GLN
5	E	43	GLN
5	E	52	ASN
5	E	61	GLN
5	E	86	HIS
5	E	120	ASN
5	E	141	GLN
5	E	177	GLN
5	E	222	ASN
5	E	235	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
7	SO4	B	103	-	4,4,4	0.28	0	6,6,6	0.07	0
6	GOL	E	247	-	5,5,5	0.77	0	5,5,5	0.23	0
6	GOL	A	278	-	5,5,5	0.55	0	5,5,5	0.27	0
6	GOL	D	6	-	5,5,5	0.61	0	5,5,5	0.21	0
6	GOL	B	101	-	5,5,5	0.47	0	5,5,5	0.16	0
7	SO4	E	252	-	4,4,4	0.27	0	6,6,6	0.08	0
7	SO4	A	281	-	4,4,4	0.31	0	6,6,6	0.13	0
8	MES	B	100	-	12,12,12	2.14	1 (8%)	15,16,16	2.31	6 (40%)
7	SO4	A	280	-	4,4,4	0.23	0	6,6,6	0.13	0
6	GOL	A	277	-	5,5,5	0.56	0	5,5,5	0.15	0
7	SO4	B	102	-	4,4,4	0.24	0	6,6,6	0.09	0
6	GOL	E	250	-	5,5,5	0.45	0	5,5,5	0.32	0
7	SO4	E	253	-	4,4,4	0.23	0	6,6,6	0.11	0
6	GOL	E	1	-	5,5,5	0.47	0	5,5,5	0.22	0
6	GOL	A	279	-	5,5,5	0.49	0	5,5,5	0.19	0
6	GOL	E	248	-	5,5,5	0.48	0	5,5,5	0.30	0
7	SO4	E	251	-	4,4,4	0.26	0	6,6,6	0.04	0
6	GOL	D	202	-	5,5,5	0.64	0	5,5,5	0.20	0
6	GOL	E	249	-	5,5,5	0.67	0	5,5,5	0.22	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
6	GOL	A	279	-	-	1/4/4/4	-
6	GOL	E	248	-	-	2/4/4/4	-
6	GOL	E	247	-	-	3/4/4/4	-
6	GOL	A	278	-	-	0/4/4/4	-
6	GOL	D	6	-	-	4/4/4/4	-
6	GOL	E	250	-	-	2/4/4/4	-
8	MES	B	100	-	-	5/6/14/14	0/1/1/1
6	GOL	B	101	-	-	4/4/4/4	-
6	GOL	D	202	-	-	2/4/4/4	-
6	GOL	E	249	-	-	4/4/4/4	-
6	GOL	E	1	-	-	2/4/4/4	-
6	GOL	A	277	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	100	MES	C8-S	-6.88	1.67	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	100	MES	C5-N4-C3	4.82	119.22	108.84
8	B	100	MES	C7-N4-C5	3.55	120.70	111.24
8	B	100	MES	C7-N4-C3	3.32	120.07	111.24
8	B	100	MES	C6-C5-N4	-2.86	105.77	110.12
8	B	100	MES	C2-C3-N4	-2.64	106.11	110.12
8	B	100	MES	O1S-S-C8	2.35	110.27	106.73

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	101	GOL	C1-C2-C3-O3
6	E	1	GOL	C1-C2-C3-O3
6	E	247	GOL	O1-C1-C2-C3
6	E	248	GOL	O1-C1-C2-C3
6	E	249	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	E	249	GOL	C1-C2-C3-O3
6	E	249	GOL	O2-C2-C3-O3
6	E	250	GOL	O1-C1-C2-C3
8	B	100	MES	C8-C7-N4-C5
8	B	100	MES	C7-C8-S-O3S
6	A	277	GOL	O1-C1-C2-C3
6	A	277	GOL	C1-C2-C3-O3
6	B	101	GOL	O1-C1-C2-C3
6	D	6	GOL	O1-C1-C2-C3
6	D	6	GOL	C1-C2-C3-O3
6	D	202	GOL	C1-C2-C3-O3
6	B	101	GOL	O1-C1-C2-O2
6	D	202	GOL	O2-C2-C3-O3
6	E	247	GOL	O1-C1-C2-O2
6	E	248	GOL	O1-C1-C2-O2
6	E	249	GOL	O1-C1-C2-O2
8	B	100	MES	N4-C7-C8-S
6	B	101	GOL	O2-C2-C3-O3
6	E	250	GOL	O1-C1-C2-O2
6	A	277	GOL	O1-C1-C2-O2
6	A	277	GOL	O2-C2-C3-O3
6	E	1	GOL	O2-C2-C3-O3
8	B	100	MES	C7-C8-S-O1S
8	B	100	MES	C7-C8-S-O2S
6	E	247	GOL	C1-C2-C3-O3
6	D	6	GOL	O2-C2-C3-O3
6	D	6	GOL	O1-C1-C2-O2
6	A	279	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	247	GOL	3	0
6	A	278	GOL	2	0
6	D	6	GOL	3	0
6	B	101	GOL	1	0
7	B	102	SO4	1	0
6	E	250	GOL	5	0
6	E	1	GOL	1	0
6	A	279	GOL	3	0
6	D	202	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	249	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, 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	276/276 (100%)	0.19	11 (3%) 42 43	6, 20, 60, 76	0
2	B	100/100 (100%)	0.52	6 (6%) 27 27	11, 30, 58, 63	0
3	C	9/9 (100%)	-0.08	0 100 100	7, 11, 19, 21	0
4	D	195/195 (100%)	0.89	27 (13%) 6 5	10, 32, 66, 76	0
5	E	245/245 (100%)	0.16	5 (2%) 65 65	7, 18, 43, 60	0
All	All	825/825 (100%)	0.38	49 (5%) 28 27	6, 24, 59, 76	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	8	SER	5.0
4	D	191	ILE	4.8
4	D	42	ALA	4.4
4	D	70	ASP	4.3
4	D	59	ASP	4.2
4	D	125	SER	3.5
4	D	201	PRO	3.5
1	A	195	SER	3.5
4	D	128	SER	3.4
2	B	99	MET	3.2
5	E	43	GLN	3.0
4	D	180	ASP	2.9
2	B	97	ARG	2.9
4	D	130	LYS	2.9
4	D	7	GLN	2.8
1	A	194	VAL	2.8
4	D	126	LYS	2.8
4	D	183	CYS	2.8
5	E	40	PHE	2.7
5	E	41	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	192	HIS	2.6
4	D	190	SER	2.5
2	B	98	ASP	2.5
4	D	193	PRO	2.5
4	D	66	LEU	2.5
4	D	127	SER	2.5
1	A	225	THR	2.4
4	D	76	ARG	2.4
4	D	10	PHE	2.4
1	A	276	PRO	2.3
1	A	252	GLY	2.3
1	A	197	HIS	2.3
4	D	131	SER	2.3
2	B	1	ILE	2.3
5	E	75	LEU	2.3
4	D	188	ASN	2.2
5	E	65	LYS	2.2
4	D	124	ASP	2.2
1	A	196	ASP	2.2
1	A	193	ALA	2.2
1	A	275	GLU	2.2
4	D	194	GLU	2.2
4	D	148	LYS	2.2
4	D	197	PHE	2.2
4	D	200	SER	2.1
2	B	0	MET	2.1
2	B	16	GLU	2.1
4	D	129	ASP	2.1
1	A	227	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

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
7	SO4	B	103	5/5	0.21	0.18	99,99,100,100	0
8	MES	B	100	12/12	0.40	0.32	97,98,100,100	0
6	GOL	D	6	6/6	0.49	0.25	57,58,58,59	0
6	GOL	B	101	6/6	0.66	0.17	63,63,63,63	0
6	GOL	E	249	6/6	0.69	0.26	45,50,51,51	0
6	GOL	A	277	6/6	0.70	0.16	36,37,39,41	0
7	SO4	E	252	5/5	0.73	0.23	77,79,79,80	0
6	GOL	A	278	6/6	0.73	0.16	37,39,41,43	0
6	GOL	E	250	6/6	0.76	0.23	41,44,45,46	0
6	GOL	E	1	6/6	0.76	0.18	52,55,56,56	0
6	GOL	A	279	6/6	0.79	0.17	48,52,52,52	0
6	GOL	E	247	6/6	0.79	0.20	22,29,31,34	0
7	SO4	B	102	5/5	0.79	0.16	70,71,72,72	0
7	SO4	E	253	5/5	0.80	0.16	64,65,66,67	0
6	GOL	E	248	6/6	0.81	0.14	56,58,58,58	0
7	SO4	A	281	5/5	0.83	0.12	66,67,67,68	0
6	GOL	D	202	6/6	0.85	0.26	46,50,52,54	0
7	SO4	A	280	5/5	0.88	0.10	47,48,52,52	0
7	SO4	E	251	5/5	0.92	0.11	55,55,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.