



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:26 PM UTC

PDB ID : 3S5L / pdb_00003s5l
Title : Crystal structure of CD4 mutant bound to HLA-DR1
Authors : Li, Y.
Deposited on : 2011-05-23
Resolution : 2.10 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

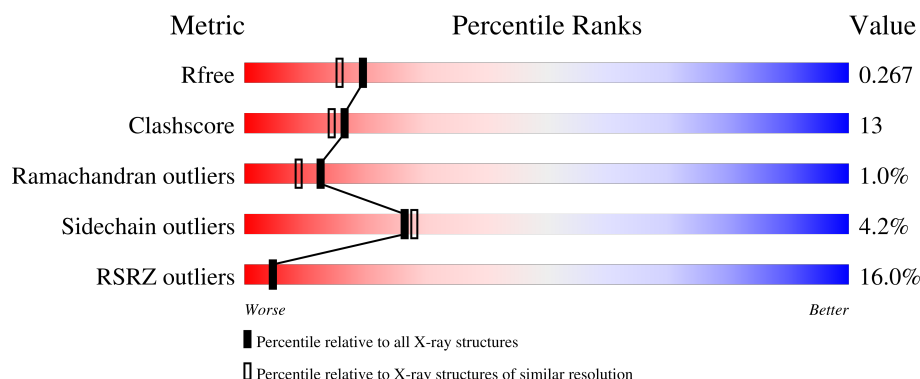
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	182	3% 81% 15% ..
1	D	182	9% 74% 22% ...
2	B	193	7% 76% 21% ..
2	E	193	13% 68% 28% ..
3	C	13	15% 62% 31% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	13	23% 54% 31% 15%
4	G	191	24% 58% 30% • • 8%
4	H	191	35% 59% 30% • 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9272 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1464	949	237	273	5			
1	D	179	Total	C	N	O	S	0	0	0
			1467	950	238	274	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLN	HIS	conflict	UNP P01903
D	177	GLN	HIS	conflict	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen DR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	191	Total	C	N	O	S	0	0	0
			1533	961	275	290	7			
2	E	191	Total	C	N	O	S	0	0	0
			1545	971	276	291	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP D7RIG0
E	0	MET	-	initiating methionine	UNP D7RIG0

- Molecule 3 is a protein called HA peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			106	69	18	19			
3	F	13	Total	C	N	O	0	0	0
			106	69	18	19			

- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	175	Total	C	N	O	S	0	0	0
			1369	860	244	261	4			
4	H	177	Total	C	N	O	S	0	0	0
			1354	851	241	258	4			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	ASP	-	expression tag	UNP P01730
G	-2	LEU	-	expression tag	UNP P01730
G	-1	GLY	-	expression tag	UNP P01730
G	0	SER	-	expression tag	UNP P01730
G	40	TYR	GLN	engineered mutation	UNP P01730
G	45	TRP	THR	engineered mutation	UNP P01730
G	60	ARG	SER	engineered mutation	UNP P01730
G	63	ARG	ASP	engineered mutation	UNP P01730
G	179	ALA	-	expression tag	UNP P01730
G	180	ALA	-	expression tag	UNP P01730
G	181	ALA	-	expression tag	UNP P01730
G	182	HIS	-	expression tag	UNP P01730
G	183	HIS	-	expression tag	UNP P01730
G	184	HIS	-	expression tag	UNP P01730
G	185	HIS	-	expression tag	UNP P01730
G	186	HIS	-	expression tag	UNP P01730
G	187	HIS	-	expression tag	UNP P01730
H	-3	ASP	-	expression tag	UNP P01730
H	-2	LEU	-	expression tag	UNP P01730
H	-1	GLY	-	expression tag	UNP P01730
H	0	SER	-	expression tag	UNP P01730
H	40	TYR	GLN	engineered mutation	UNP P01730
H	45	TRP	THR	engineered mutation	UNP P01730
H	60	ARG	SER	engineered mutation	UNP P01730
H	63	ARG	ASP	engineered mutation	UNP P01730
H	179	ALA	-	expression tag	UNP P01730
H	180	ALA	-	expression tag	UNP P01730
H	181	ALA	-	expression tag	UNP P01730
H	182	HIS	-	expression tag	UNP P01730
H	183	HIS	-	expression tag	UNP P01730
H	184	HIS	-	expression tag	UNP P01730
H	185	HIS	-	expression tag	UNP P01730
H	186	HIS	-	expression tag	UNP P01730
H	187	HIS	-	expression tag	UNP P01730

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	G	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	87	Total	O	0	0
			87	87		

Continued on next page...

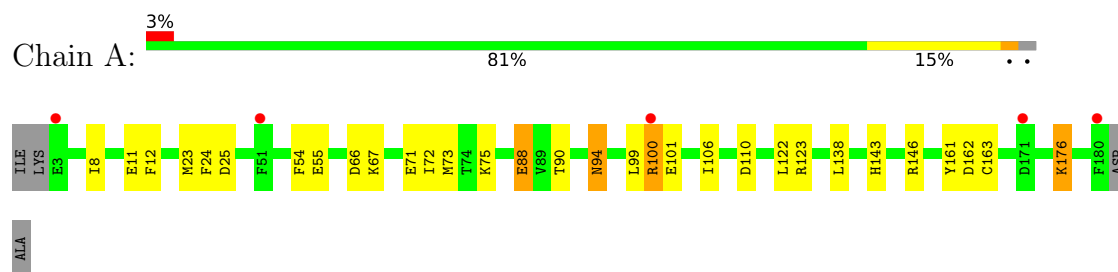
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	61	Total 61	O 61	0	0
6	B	57	Total 57	O 57	0	0
6	E	30	Total 30	O 30	0	0
6	C	5	Total 5	O 5	0	0
6	F	1	Total 1	O 1	0	0
6	G	16	Total 16	O 16	0	0
6	H	11	Total 11	O 11	0	0

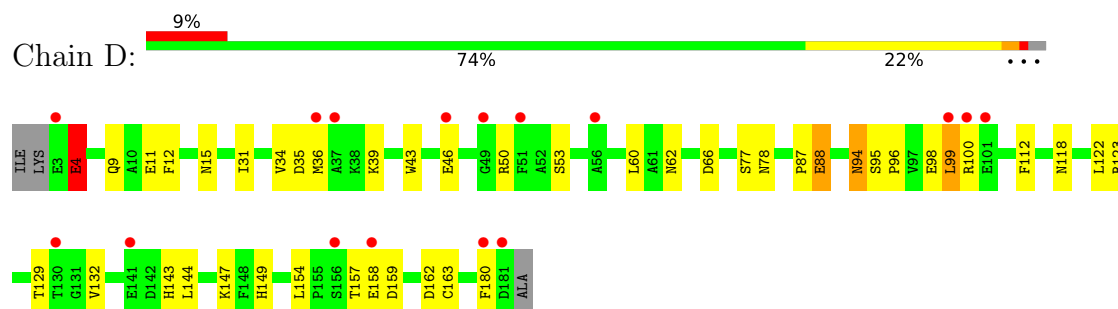
3 Residue-property plots [i](#)

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.

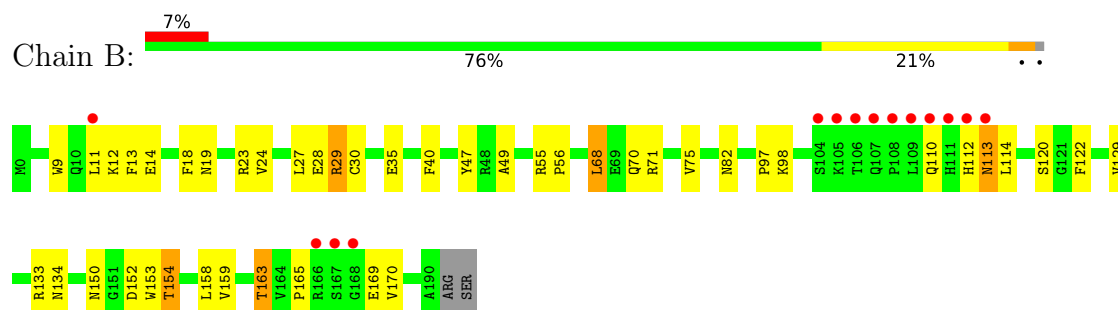
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



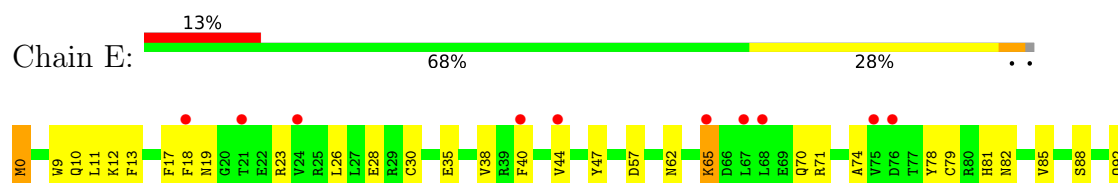
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



- Molecule 2: HLA class II histocompatibility antigen DR beta chain

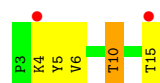


- Molecule 2: HLA class II histocompatibility antigen DR beta chain

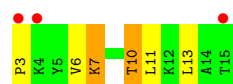




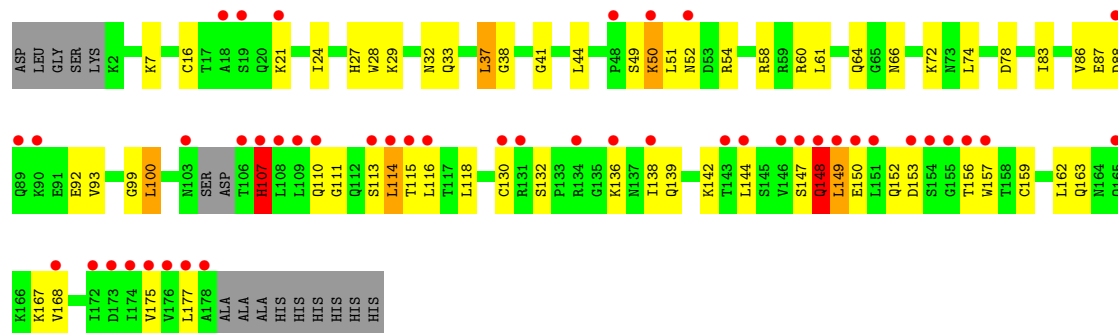
- Molecule 3: HA peptide



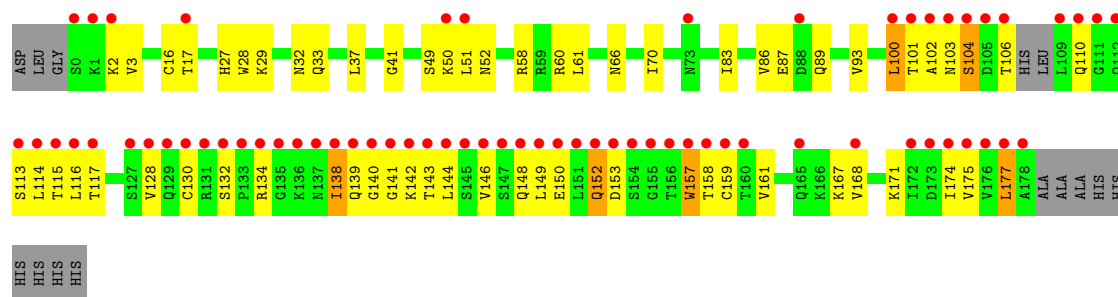
- Molecule 3: HA peptide



- Molecule 4: T-cell surface glycoprotein CD4



- Molecule 4: T-cell surface glycoprotein CD4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.20Å 119.70Å 137.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.10) 99.9 (50.00-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.10Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.268 0.233 , 0.267	Depositor DCC
R_{free} test set	4566 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtrriage
Anisotropy	0.793	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9272	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.21 % 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 1.8222e-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: GOL

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	0.59	0/1508	1.02	6/2056 (0.3%)
1	D	0.56	0/1511	0.99	7/2060 (0.3%)
2	B	0.56	0/1571	0.97	4/2130 (0.2%)
2	E	0.52	0/1584	0.93	4/2150 (0.2%)
3	C	0.52	0/107	1.01	0/141
3	F	0.41	0/107	0.96	0/141
4	G	0.42	0/1390	0.91	4/1873 (0.2%)
4	H	0.46	0/1374	0.94	2/1854 (0.1%)
All	All	0.53	0/9152	0.96	27/12405 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	GLU	N-CA-C	-7.84	96.90	109.76
1	D	163	CYS	N-CA-C	-7.46	96.37	108.52
1	D	88	GLU	N-CA-C	-6.92	98.34	109.96
1	A	163	CYS	N-CA-C	-6.80	97.43	108.52
1	A	138	LEU	CA-C-N	6.78	126.70	119.85
1	A	138	LEU	C-N-CA	6.78	126.70	119.85
1	D	159	ASP	N-CA-C	6.56	119.75	110.50
1	D	31	ILE	N-CA-C	-6.48	104.53	110.82
2	B	98	LYS	N-CA-C	-6.45	98.72	109.24
4	G	41	GLY	N-CA-C	-6.45	98.99	110.86
2	B	120	SER	N-CA-C	6.24	118.44	109.14
1	D	144	LEU	N-CA-C	-6.20	100.25	109.86
1	A	101	GLU	CA-C-N	6.09	126.11	119.90
1	A	101	GLU	C-N-CA	6.09	126.11	119.90
2	E	122	PHE	N-CA-C	6.04	119.78	110.42
2	E	98	LYS	N-CA-C	-5.79	99.80	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	163	THR	N-CA-C	5.58	117.55	109.07
1	D	154	LEU	CA-C-N	5.58	125.90	119.93
1	D	154	LEU	C-N-CA	5.58	125.90	119.93
4	G	78	ASP	N-CA-C	-5.53	106.04	112.89
4	H	41	GLY	N-CA-C	-5.53	100.69	110.86
4	H	117	THR	N-CA-C	5.48	118.75	109.76
4	G	142	LYS	N-CA-C	-5.28	105.94	112.38
2	E	35	GLU	N-CA-C	5.18	116.96	108.52
4	G	74	LEU	N-CA-C	5.15	117.50	110.24
2	B	35	GLU	N-CA-C	5.13	116.88	108.52
2	E	44	VAL	N-CA-C	-5.08	107.44	111.81

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	1464	0	1404	25	0
1	D	1467	0	1403	29	0
2	B	1533	0	1442	36	0
2	E	1545	0	1466	44	0
3	C	106	0	119	12	0
3	F	106	0	119	6	0
4	G	1369	0	1385	52	0
4	H	1354	0	1339	53	0
5	A	6	0	8	0	0
5	B	12	0	16	0	0
5	D	6	0	8	0	0
5	E	18	0	24	1	0
5	G	12	0	16	3	0
5	H	6	0	8	3	0
6	A	87	0	0	1	0
6	B	57	0	0	0	0
6	C	5	0	0	0	0
6	D	61	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	30	0	0	1	0
6	F	1	0	0	0	0
6	G	16	0	0	0	0
6	H	11	0	0	0	0
All	All	9272	0	8757	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (229) 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:50:LYS:H	4:H:50:LYS:HD2	1.07	1.13
4:G:50:LYS:HE3	4:G:50:LYS:H	1.12	1.04
4:H:177:LEU:HD22	4:H:177:LEU:H	1.23	1.01
4:G:138:ILE:HG22	4:G:139:GLN:H	1.28	0.99
2:E:82:ASN:HD21	3:F:6:VAL:H	1.08	0.93
1:A:55:GLU:H	3:C:4:LYS:HE3	1.31	0.93
4:H:50:LYS:HD2	4:H:50:LYS:N	1.85	0.91
4:G:50:LYS:HE3	4:G:50:LYS:N	1.91	0.86
1:D:147:LYS:HE3	1:D:149:HIS:HE1	1.40	0.85
1:A:55:GLU:N	3:C:4:LYS:HE3	1.91	0.84
2:B:150:ASN:HD22	2:B:154:THR:CG2	1.91	0.83
4:H:27:HIS:NE2	4:H:29:LYS:HE3	1.95	0.82
2:E:85:VAL:HG13	3:F:3:PRO:HB2	1.62	0.81
1:D:4:GLU:HB3	2:E:17:PHE:O	1.80	0.81
4:H:115:THR:HG23	4:H:116:LEU:H	1.44	0.81
4:H:60:ARG:HH21	5:H:964:GOL:H32	1.46	0.79
2:B:82:ASN:HD21	3:C:6:VAL:H	1.28	0.78
4:H:102:ALA:HA	4:H:116:LEU:HA	1.67	0.77
4:G:60:ARG:NH2	5:G:965:GOL:H2	1.99	0.76
1:A:54:PHE:HA	3:C:4:LYS:CE	2.16	0.75
2:E:47:TYR:H	2:E:62:ASN:HD21	1.33	0.75
4:H:50:LYS:H	4:H:50:LYS:CD	1.90	0.74
4:G:50:LYS:H	4:G:50:LYS:CE	1.96	0.74
2:B:150:ASN:HD22	2:B:154:THR:HG23	1.49	0.74
2:B:113:ASN:ND2	2:B:114:LEU:H	1.88	0.72
4:G:138:ILE:HG22	4:G:139:GLN:N	2.02	0.72
4:H:177:LEU:HD22	4:H:177:LEU:N	2.02	0.72
4:G:37:LEU:HG	4:G:44:LEU:HD11	1.73	0.71
4:H:115:THR:HG23	4:H:116:LEU:N	2.07	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:132:SER:OG	4:G:136:LYS:HG2	1.92	0.69
4:H:132:SER:HA	4:H:157:TRP:NE1	2.08	0.68
1:A:66:ASP:OD1	3:C:10:THR:HG21	1.93	0.68
2:B:11:LEU:CD2	3:C:10:THR:HG23	2.23	0.68
4:H:58:ARG:HG3	4:H:70:ILE:CD1	2.24	0.68
2:B:13:PHE:CE2	2:B:28:GLU:HG3	2.29	0.67
4:H:60:ARG:NH2	5:H:964:GOL:H32	2.11	0.65
2:E:18:PHE:HB2	2:E:23:ARG:HB3	1.79	0.64
4:H:132:SER:HA	4:H:157:TRP:CD1	2.34	0.63
4:H:158:THR:HG22	4:H:171:LYS:HG2	1.79	0.63
2:E:98:LYS:HD2	2:E:98:LYS:N	2.12	0.62
2:B:163:THR:HG23	2:B:165:PRO:HD3	1.81	0.62
2:B:70:GLN:NE2	2:B:71:ARG:HH21	1.96	0.62
1:A:54:PHE:HA	3:C:4:LYS:HE3	1.82	0.61
4:H:177:LEU:H	4:H:177:LEU:CD2	2.04	0.61
4:H:106:THR:HA	4:H:177:LEU:HD21	1.81	0.61
2:B:112:HIS:O	2:B:113:ASN:HB2	2.02	0.60
2:B:134:ASN:ND2	2:B:170:VAL:H	2.00	0.60
2:E:88:SER:HA	2:E:92:GLN:NE2	2.17	0.60
4:G:138:ILE:CG2	4:G:139:GLN:H	2.09	0.59
4:H:157:TRP:HZ3	4:H:174:ILE:HB	1.67	0.59
4:G:99:GLY:O	4:G:118:LEU:HD12	2.02	0.58
4:G:27:HIS:NE2	4:G:29:LYS:HE3	2.17	0.58
1:A:54:PHE:HA	3:C:4:LYS:HE2	1.85	0.58
1:D:94:ASN:HD22	1:D:94:ASN:N	2.01	0.58
2:E:70:GLN:HE22	2:E:71:ARG:HD2	1.67	0.58
2:B:150:ASN:HB2	2:B:154:THR:HG22	1.86	0.58
2:B:70:GLN:HE22	2:B:71:ARG:HH21	1.51	0.57
4:G:114:LEU:HB2	4:G:149:LEU:HD21	1.85	0.57
4:G:114:LEU:HD22	4:G:115:THR:N	2.20	0.57
1:D:94:ASN:HD22	1:D:94:ASN:H	1.53	0.57
4:H:110:GLN:O	4:H:149:LEU:HB2	2.05	0.56
4:G:147:SER:C	4:G:148:GLN:HG2	2.31	0.56
2:B:27:LEU:HG	2:B:29:ARG:HD2	1.88	0.56
2:E:134:ASN:ND2	2:E:170:VAL:H	2.04	0.56
1:A:110:ASP:OD2	1:A:146:ARG:HG2	2.06	0.56
1:D:87:PRO:HB3	1:D:112:PHE:HB3	1.86	0.56
4:G:162:LEU:C	4:G:162:LEU:HD13	2.31	0.56
1:D:118:ASN:HD22	2:E:0:MET:HG2	1.71	0.55
4:G:58:ARG:HD2	5:G:965:GOL:O2	2.05	0.55
4:H:115:THR:CG2	4:H:116:LEU:H	2.16	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:60:ARG:HH21	5:G:965:GOL:H2	1.70	0.55
3:C:4:LYS:HE2	3:C:5:TYR:O	2.07	0.55
4:G:113:SER:OG	4:G:147:SER:HA	2.07	0.55
2:E:65:LYS:NZ	2:E:65:LYS:HB2	2.22	0.55
2:E:11:LEU:N	2:E:11:LEU:HD22	2.22	0.54
2:E:74:ALA:O	2:E:78:TYR:HB3	2.07	0.54
1:D:34:VAL:O	1:D:36:MET:HE2	2.07	0.54
1:D:143:HIS:HD2	2:E:12:LYS:NZ	2.06	0.54
2:B:113:ASN:HD22	2:B:114:LEU:H	1.54	0.54
4:H:157:TRP:CZ3	4:H:174:ILE:HB	2.43	0.54
2:B:9:TRP:CH2	2:B:30:CYS:HB3	2.42	0.54
2:E:19:ASN:C	2:E:19:ASN:HD22	2.17	0.53
1:A:90:THR:HG23	6:A:187:HOH:O	2.07	0.53
4:G:100:LEU:HD21	4:G:116:LEU:HB3	1.89	0.53
2:E:81:HIS:O	2:E:85:VAL:HG23	2.09	0.53
2:E:163:THR:HG23	2:E:165:PRO:HD3	1.91	0.53
2:E:40:PHE:HB2	2:E:47:TYR:CE1	2.44	0.52
4:G:87:GLU:O	4:G:87:GLU:HG3	2.09	0.52
1:D:12:PHE:CD1	1:D:12:PHE:C	2.87	0.52
2:B:133:ARG:NH2	2:B:169:GLU:OE1	2.40	0.52
4:G:61:LEU:HB3	4:G:66:ASN:HB2	1.92	0.52
1:A:88:GLU:HG3	4:G:60:ARG:HG3	1.92	0.51
2:E:130:ARG:NH1	2:E:176:GLU:OE1	2.42	0.51
4:G:83:ILE:HG13	4:G:92:GLU:HG2	1.92	0.51
2:B:152:ASP:OD1	2:B:154:THR:HG22	2.10	0.51
1:A:72:ILE:HD13	3:C:15:THR:HG22	1.91	0.51
1:D:66:ASP:OD1	3:F:10:THR:HG21	2.11	0.51
4:G:21:LYS:HG2	4:G:64:GLN:O	2.11	0.51
4:G:7:LYS:CG	4:G:168:VAL:HG21	2.41	0.51
4:H:114:LEU:N	4:H:146:VAL:O	2.43	0.51
4:H:175:VAL:HG23	4:H:175:VAL:O	2.10	0.50
1:D:11:GLU:HG3	2:E:11:LEU:HB2	1.93	0.50
2:E:70:GLN:NE2	2:E:71:ARG:HD2	2.26	0.50
2:B:11:LEU:HD22	3:C:10:THR:HG23	1.92	0.50
4:G:156:THR:HG23	4:G:156:THR:O	2.11	0.50
4:H:143:THR:O	4:H:144:LEU:C	2.54	0.50
4:H:100:LEU:C	4:H:100:LEU:HD23	2.36	0.50
2:B:24:VAL:CG1	2:B:75:VAL:HG23	2.42	0.50
4:H:86:VAL:O	4:H:89:GLN:HB3	2.12	0.49
2:E:134:ASN:HD21	2:E:169:GLU:HA	1.78	0.49
4:G:144:LEU:C	4:G:144:LEU:HD23	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:139:GLN:HE21	4:H:140:GLY:H	1.61	0.49
2:E:108:PRO:HG2	2:E:109:LEU:H	1.76	0.49
4:H:60:ARG:HH22	5:H:964:GOL:H12	1.77	0.49
4:G:162:LEU:HD13	4:G:163:GLN:N	2.28	0.49
4:H:161:VAL:HB	4:H:168:VAL:CG1	2.42	0.49
2:E:157:THR:C	2:E:158:LEU:HD12	2.38	0.48
1:D:118:ASN:ND2	2:E:0:MET:HG2	2.28	0.48
4:G:175:VAL:O	4:G:175:VAL:HG13	2.13	0.48
4:H:83:ILE:HD12	4:H:83:ILE:N	2.29	0.48
4:H:51:LEU:O	4:H:52:ASN:C	2.57	0.48
1:A:73:MET:HG3	2:B:9:TRP:CZ3	2.49	0.48
1:D:123:ARG:HH21	1:D:123:ARG:HG2	1.79	0.48
2:E:26:LEU:HD13	2:E:79:CYS:SG	2.54	0.48
2:B:40:PHE:HB2	2:B:47:TYR:CE1	2.48	0.47
2:E:133:ARG:NH1	2:E:169:GLU:OE1	2.47	0.47
1:D:129:THR:O	1:D:132:VAL:HG22	2.14	0.47
1:D:147:LYS:HE3	1:D:149:HIS:CE1	2.32	0.47
2:B:14:GLU:OE1	2:B:29:ARG:NH1	2.46	0.47
4:H:2:LYS:NZ	4:H:3:VAL:H	2.12	0.47
2:B:24:VAL:HB	2:B:75:VAL:CG2	2.44	0.47
2:B:70:GLN:HE22	2:B:71:ARG:HD2	1.79	0.47
1:A:123:ARG:HG3	1:A:161:TYR:CE2	2.50	0.47
4:G:51:LEU:O	4:G:52:ASN:C	2.58	0.47
4:G:24:ILE:HD11	4:G:86:VAL:HG22	1.97	0.47
4:H:100:LEU:C	4:H:100:LEU:CD2	2.88	0.47
1:A:75:LYS:HB2	1:A:75:LYS:HE3	1.66	0.46
2:E:110:GLN:C	2:E:112:HIS:H	2.23	0.46
2:E:170:VAL:HG22	2:E:189:ARG:HE	1.80	0.46
4:H:16:CYS:HB2	4:H:28:TRP:CZ2	2.50	0.46
1:A:54:PHE:CA	3:C:4:LYS:HE3	2.45	0.46
4:G:132:SER:HG	4:G:136:LYS:HG2	1.78	0.46
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.97	0.46
1:D:99:LEU:HD13	1:D:180:PHE:CE2	2.51	0.46
2:E:13:PHE:CE2	2:E:28:GLU:HG3	2.51	0.46
2:E:93:ARG:HD3	2:E:123:TYR:CD1	2.51	0.46
4:G:177:LEU:N	4:G:177:LEU:HD22	2.31	0.46
2:B:113:ASN:ND2	2:B:114:LEU:N	2.62	0.45
1:A:94:ASN:HB3	1:A:106:ILE:HD11	1.98	0.45
4:H:86:VAL:HG22	4:H:87:GLU:HG3	1.97	0.45
2:B:18:PHE:HB2	2:B:23:ARG:HB3	1.98	0.45
4:G:32:ASN:O	4:G:33:GLN:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:54:ARG:HA	4:G:72:LYS:HE2	1.98	0.45
4:H:93:VAL:HG13	4:H:93:VAL:O	2.15	0.45
4:G:38:GLY:O	4:G:44:LEU:HD12	2.17	0.45
4:H:61:LEU:HB3	4:H:66:ASN:HB2	1.99	0.45
2:B:19:ASN:HD22	2:B:19:ASN:C	2.24	0.44
4:H:157:TRP:CZ3	4:H:174:ILE:HD12	2.51	0.44
1:D:35:ASP:OD2	1:D:35:ASP:C	2.61	0.44
2:E:81:HIS:CD2	3:F:6:VAL:HG23	2.53	0.44
4:G:107:HIS:ND1	4:G:107:HIS:N	2.65	0.44
1:A:12:PHE:CD1	1:A:12:PHE:C	2.96	0.44
1:D:122:LEU:HB2	1:D:162:ASP:HB2	2.00	0.44
1:D:143:HIS:HE1	6:E:195:HOH:O	2.00	0.44
4:H:130:CYS:HA	4:H:159:CYS:HA	1.99	0.44
1:D:62:ASN:OD1	3:F:7:LYS:HE2	2.18	0.44
4:H:37:LEU:C	4:H:37:LEU:HD12	2.43	0.44
4:G:148:GLN:HE21	4:G:148:GLN:HB3	1.52	0.44
1:A:176:LYS:HD2	1:A:176:LYS:HA	1.77	0.43
2:E:107:GLN:HE21	2:E:107:GLN:HA	1.82	0.43
4:G:27:HIS:CD2	4:G:29:LYS:HE3	2.53	0.43
4:G:86:VAL:O	4:G:87:GLU:C	2.60	0.43
1:D:88:GLU:HG3	4:H:60:ARG:HG3	2.00	0.43
4:G:24:ILE:HD11	4:G:86:VAL:CG2	2.48	0.43
4:G:58:ARG:NH2	4:G:61:LEU:HD11	2.33	0.43
4:H:103:ASN:O	4:H:104:SER:CB	2.66	0.43
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.85	0.43
4:G:130:CYS:HA	4:G:159:CYS:HA	2.01	0.43
1:A:23:MET:HE1	1:A:25:ASP:HB3	2.01	0.43
1:A:67:LYS:O	1:A:71:GLU:HG2	2.19	0.43
1:A:11:GLU:HG3	2:B:11:LEU:HB3	2.01	0.43
1:D:39:LYS:HD3	1:D:60:LEU:HD21	1.99	0.43
2:E:129:VAL:HB	2:E:159:VAL:HG21	2.01	0.43
4:H:157:TRP:O	4:H:171:LYS:HA	2.18	0.43
1:A:122:LEU:HB2	1:A:162:ASP:HB2	2.00	0.43
2:E:107:GLN:HA	2:E:107:GLN:NE2	2.33	0.42
2:E:128:GLU:HG3	5:E:960:GOL:H12	2.00	0.42
2:E:104:SER:O	2:E:107:GLN:HG2	2.19	0.42
4:H:128:VAL:HG12	4:H:141:GLY:HA2	2.01	0.42
4:H:138:ILE:HG23	4:H:138:ILE:O	2.19	0.42
1:A:8:ILE:HB	1:A:25:ASP:OD2	2.20	0.42
4:H:58:ARG:HG3	4:H:70:ILE:HD11	2.01	0.42
2:E:57:ASP:CG	3:F:13:LEU:HD22	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:PRO:HB3	2:E:122:PHE:HB3	2.02	0.42
1:D:99:LEU:HA	1:D:99:LEU:HD12	1.69	0.42
4:H:141:GLY:O	4:H:142:LYS:CB	2.68	0.42
2:E:18:PHE:O	2:E:19:ASN:C	2.63	0.42
4:G:150:GLU:O	4:G:153:ASP:HB2	2.20	0.42
1:D:9:GLN:HB3	2:E:13:PHE:HB2	2.00	0.42
1:A:99:LEU:O	1:A:100:ARG:HG2	2.19	0.42
2:B:55:ARG:N	2:B:56:PRO:CD	2.83	0.41
1:A:8:ILE:O	1:A:24:PHE:HA	2.20	0.41
2:E:10:GLN:C	2:E:11:LEU:HD22	2.45	0.41
2:E:177:HIS:CD2	2:E:178:PRO:HD2	2.55	0.41
1:D:77:SER:O	1:D:78:ASN:HB2	2.21	0.41
2:B:129:VAL:HB	2:B:159:VAL:HG21	2.03	0.41
1:D:95:SER:HB2	1:D:96:PRO:HD2	2.02	0.41
4:G:110:GLN:HB2	4:G:177:LEU:O	2.20	0.41
2:B:28:GLU:HB3	2:B:40:PHE:HB3	2.02	0.41
2:B:49:ALA:HB2	2:B:55:ARG:HA	2.02	0.41
4:G:83:ILE:N	4:G:83:ILE:HD12	2.36	0.41
4:G:111:GLY:O	4:G:148:GLN:HA	2.20	0.41
4:H:32:ASN:O	4:H:33:GLN:HB2	2.21	0.41
4:H:157:TRP:CE3	4:H:174:ILE:HD12	2.56	0.41
1:A:143:HIS:HD2	2:B:12:LYS:NZ	2.19	0.41
4:G:132:SER:HB3	4:G:157:TRP:CH2	2.56	0.41
4:G:93:VAL:O	4:G:93:VAL:HG13	2.20	0.40
4:H:100:LEU:HD23	4:H:101:THR:N	2.36	0.40
4:H:100:LEU:HD21	4:H:116:LEU:HG	2.04	0.40
4:H:134:ARG:HD3	4:H:152:GLN:HB3	2.04	0.40
2:B:152:ASP:O	2:B:153:TRP:HB2	2.21	0.40
2:E:9:TRP:CH2	2:E:30:CYS:HB3	2.56	0.40
4:G:7:LYS:HG2	4:G:168:VAL:HG21	2.03	0.40
1:D:43:TRP:HZ2	1:D:53:SER:HA	1.86	0.40
1:D:46:GLU:OE2	1:D:50:ARG:HD3	2.22	0.40
1:D:98:GLU:O	1:D:99:LEU:C	2.62	0.40
4:G:16:CYS:HB2	4:G:28:TRP:CZ2	2.57	0.40
4:G:136:LYS:O	4:G:136:LYS:HG3	2.22	0.40
4:H:153:ASP:HB3	4:H:157:TRP:CH2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	176/182 (97%)	172 (98%)	4 (2%)	0	100	100
1	D	177/182 (97%)	170 (96%)	6 (3%)	1 (1%)	21	18
2	B	189/193 (98%)	178 (94%)	9 (5%)	2 (1%)	11	8
2	E	189/193 (98%)	176 (93%)	12 (6%)	1 (0%)	24	22
3	C	11/13 (85%)	11 (100%)	0	0	100	100
3	F	11/13 (85%)	11 (100%)	0	0	100	100
4	G	171/191 (90%)	158 (92%)	10 (6%)	3 (2%)	6	3
4	H	173/191 (91%)	151 (87%)	18 (10%)	4 (2%)	5	2
All	All	1097/1158 (95%)	1027 (94%)	59 (5%)	11 (1%)	12	9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	104	SER
4	G	148	GLN
4	H	113	SER
4	H	138	ILE
4	H	148	GLN
2	B	110	GLN
4	G	88	ASP
1	D	4	GLU
4	G	107	HIS
2	B	113	ASN
2	E	108	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	163/166 (98%)	160 (98%)	3 (2%)	51	60
1	D	163/166 (98%)	156 (96%)	7 (4%)	26	27
2	B	165/174 (95%)	161 (98%)	4 (2%)	43	49
2	E	168/174 (97%)	163 (97%)	5 (3%)	36	41
3	C	12/12 (100%)	11 (92%)	1 (8%)	10	8
3	F	12/12 (100%)	9 (75%)	3 (25%)	0	0
4	G	155/170 (91%)	145 (94%)	10 (6%)	15	13
4	H	146/170 (86%)	138 (94%)	8 (6%)	19	18
All	All	984/1044 (94%)	943 (96%)	41 (4%)	26	28

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

Mol	Chain	Res	Type
1	A	94	ASN
1	A	100	ARG
1	A	176	LYS
1	D	4	GLU
1	D	15	ASN
1	D	94	ASN
1	D	99	LEU
1	D	100	ARG
1	D	157	THR
1	D	158	GLU
2	B	29	ARG
2	B	68	LEU
2	B	154	THR
2	B	158	LEU
2	E	0	MET
2	E	38	VAL
2	E	65	LYS
2	E	113	ASN
2	E	166	ARG
3	C	10	THR
3	F	7	LYS
3	F	10	THR
3	F	11	LEU
4	G	37	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	49	SER
4	G	50	LYS
4	G	100	LEU
4	G	107	HIS
4	G	114	LEU
4	G	148	GLN
4	G	149	LEU
4	G	152	GLN
4	G	167	LYS
4	H	17	THR
4	H	49	SER
4	H	100	LEU
4	H	150	GLU
4	H	152	GLN
4	H	157	TRP
4	H	167	LYS
4	H	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	94	ASN
1	A	143	HIS
1	A	149	HIS
1	D	15	ASN
1	D	78	ASN
1	D	94	ASN
1	D	118	ASN
1	D	143	HIS
1	D	149	HIS
2	B	19	ASN
2	B	70	GLN
2	B	82	ASN
2	B	113	ASN
2	B	134	ASN
2	B	136	GLN
2	B	150	ASN
2	B	156	GLN
2	B	174	GLN
2	E	19	ASN
2	E	62	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	70	GLN
2	E	82	ASN
2	E	92	GLN
2	E	107	GLN
2	E	113	ASN
2	E	134	ASN
2	E	174	GLN
4	G	25	GLN
4	G	33	GLN
4	G	103	ASN
4	G	112	GLN
4	G	139	GLN
4	G	148	GLN
4	H	89	GLN
4	H	94	GLN
4	H	110	GLN
4	H	112	GLN
4	H	139	GLN
4	H	165	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	GOL	A	968	-	5,5,5	0.30	0	5,5,5	0.39	0
5	GOL	H	964	-	5,5,5	0.24	0	5,5,5	0.30	0
5	GOL	G	967	-	5,5,5	0.27	0	5,5,5	0.28	0
5	GOL	B	966	-	5,5,5	0.38	0	5,5,5	0.45	0
5	GOL	E	963	-	5,5,5	0.37	0	5,5,5	0.31	0
5	GOL	E	962	-	5,5,5	0.15	0	5,5,5	0.31	0
5	GOL	D	961	-	5,5,5	0.25	0	5,5,5	0.34	0
5	GOL	E	960	-	5,5,5	0.25	0	5,5,5	0.38	0
5	GOL	B	969	-	5,5,5	0.30	0	5,5,5	0.28	0
5	GOL	G	965	-	5,5,5	0.18	0	5,5,5	0.35	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	A	968	-	-	0/4/4/4	-
5	GOL	H	964	-	-	0/4/4/4	-
5	GOL	G	967	-	-	0/4/4/4	-
5	GOL	B	966	-	-	0/4/4/4	-
5	GOL	E	963	-	-	0/4/4/4	-
5	GOL	E	962	-	-	0/4/4/4	-
5	GOL	D	961	-	-	0/4/4/4	-
5	GOL	E	960	-	-	0/4/4/4	-
5	GOL	B	969	-	-	0/4/4/4	-
5	GOL	G	965	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	964	GOL	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	960	GOL	1	0
5	G	965	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	178/182 (97%)	-0.02	5 (2%) 55 57	15, 25, 44, 61	0
1	D	179/182 (98%)	0.45	16 (8%) 15 16	16, 30, 57, 68	0
2	B	191/193 (98%)	0.28	14 (7%) 21 22	16, 29, 51, 95	0
2	E	191/193 (98%)	0.84	26 (13%) 7 7	19, 36, 63, 94	0
3	C	13/13 (100%)	0.84	2 (15%) 5 5	26, 32, 39, 44	0
3	F	13/13 (100%)	1.51	3 (23%) 2 2	35, 43, 57, 58	0
4	G	175/191 (91%)	1.37	46 (26%) 1 1	25, 49, 74, 81	0
4	H	177/191 (92%)	1.56	67 (37%) 1 1	23, 45, 77, 85	0
All	All	1117/1158 (96%)	0.75	179 (16%) 5 5	15, 34, 72, 95	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	106	THR	8.0
2	E	109	LEU	7.7
4	H	178	ALA	7.6
4	G	178	ALA	6.7
2	E	111	HIS	6.5
4	H	144	LEU	6.5
4	H	114	LEU	6.3
4	H	115	THR	6.2
4	H	138	ILE	6.1
4	H	145	SER	6.1
4	H	103	ASN	5.8
4	H	105	ASP	5.6
2	E	108	PRO	5.4
4	G	108	LEU	5.2
2	E	190	ALA	5.0
2	E	110	GLN	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	112	HIS	4.7
4	G	106	THR	4.7
4	H	157	TRP	4.7
4	H	102	ALA	4.7
4	G	149	LEU	4.7
4	H	177	LEU	4.6
4	H	141	GLY	4.5
2	E	107	GLN	4.4
4	H	146	VAL	4.4
2	E	112	HIS	4.3
4	H	143	THR	4.3
4	H	136	LYS	4.3
4	G	177	LEU	4.2
4	H	147	SER	4.2
4	H	130	CYS	4.2
1	D	51	PHE	4.1
2	B	106	THR	4.1
4	G	109	LEU	4.1
4	H	113	SER	4.0
4	H	151	LEU	4.0
4	H	104	SER	4.0
4	H	158	THR	4.0
4	G	146	VAL	4.0
4	H	174	ILE	4.0
4	G	134	ARG	3.9
4	G	172	ILE	3.9
4	H	112	GLN	3.8
4	G	103	ASN	3.7
4	H	149	LEU	3.7
4	H	135	GLY	3.7
2	B	111	HIS	3.7
4	G	110	GLN	3.6
4	G	151	LEU	3.6
4	H	137	ASN	3.6
4	H	116	LEU	3.6
4	H	140	GLY	3.5
4	H	159	CYS	3.5
1	D	180	PHE	3.5
1	A	100	ARG	3.5
4	G	168	VAL	3.5
4	G	138	ILE	3.4
2	B	109	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	G	114	LEU	3.4
4	H	153	ASP	3.3
4	H	142	LYS	3.3
4	G	154	SER	3.3
4	H	111	GLY	3.3
4	G	107	HIS	3.3
4	H	109	LEU	3.2
2	B	110	GLN	3.2
4	H	139	GLN	3.2
2	E	167	SER	3.2
4	H	0	SER	3.2
4	H	156	THR	3.2
2	E	166	ARG	3.1
1	D	3	GLU	3.1
4	H	128	VAL	3.1
1	D	49	GLY	3.0
4	H	155	GLY	3.0
4	H	175	VAL	3.0
4	G	175	VAL	2.9
4	G	21	LYS	2.9
1	D	181	ASP	2.9
3	F	3	PRO	2.9
4	G	131	ARG	2.9
4	G	115	THR	2.8
4	G	113	SER	2.8
4	H	148	GLN	2.8
4	H	176	VAL	2.8
4	G	174	ILE	2.8
4	H	133	PRO	2.8
4	H	132	SER	2.8
2	E	68	LEU	2.8
4	G	156	THR	2.8
4	G	176	VAL	2.8
2	E	168	GLY	2.8
2	E	67	LEU	2.8
2	E	75	VAL	2.8
2	B	107	GLN	2.7
4	H	88	ASP	2.7
4	H	100	LEU	2.7
1	D	37	ALA	2.7
2	E	181	THR	2.7
4	H	131	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	101	THR	2.7
4	H	160	THR	2.7
4	H	172	ILE	2.7
4	H	50	LYS	2.6
3	F	15	THR	2.6
2	B	108	PRO	2.6
4	G	116	LEU	2.6
4	H	165	GLN	2.6
1	D	158	GLU	2.6
4	G	157	TRP	2.6
4	H	117	THR	2.6
1	A	180	PHE	2.6
4	H	168	VAL	2.5
4	G	88	ASP	2.5
4	G	153	ASP	2.5
1	D	100	ARG	2.5
1	D	130	THR	2.5
4	G	143	THR	2.5
4	H	134	ARG	2.5
2	E	44	VAL	2.4
1	D	46	GLU	2.4
4	G	130	CYS	2.4
4	G	144	LEU	2.4
2	B	168	GLY	2.4
4	G	52	ASN	2.4
4	H	150	GLU	2.4
4	H	127	SER	2.4
2	B	105	LYS	2.4
4	G	150	GLU	2.4
1	D	56	ALA	2.4
2	B	166	ARG	2.4
4	H	110	GLN	2.3
2	E	189	ARG	2.3
4	G	18	ALA	2.3
4	H	173	ASP	2.3
2	E	105	LYS	2.3
2	E	164	VAL	2.3
1	A	171	ASP	2.3
1	D	156	SER	2.3
4	G	89	GLN	2.3
2	E	21	THR	2.3
4	G	50	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	11	LEU	2.3
4	G	165	GLN	2.2
2	B	167	SER	2.2
2	E	113	ASN	2.2
4	H	51	LEU	2.2
4	H	154	SER	2.2
4	H	1	LYS	2.2
3	C	15	THR	2.2
2	E	24	VAL	2.2
4	H	152	GLN	2.2
4	H	17	THR	2.2
1	D	101	GLU	2.1
4	G	155	GLY	2.1
3	F	4	LYS	2.1
4	G	90	LYS	2.1
2	B	104	SER	2.1
4	G	19	SER	2.1
1	D	36	MET	2.1
2	B	113	ASN	2.1
4	G	147	SER	2.1
1	D	141	GLU	2.1
4	G	148	GLN	2.1
2	E	65	LYS	2.1
4	G	136	LYS	2.1
4	H	2	LYS	2.1
1	A	51	PHE	2.1
2	E	18	PHE	2.1
2	E	40	PHE	2.1
2	E	163	THR	2.0
4	G	48	PRO	2.0
1	A	3	GLU	2.0
4	H	73	ASN	2.0
1	D	99	LEU	2.0
4	H	129	GLN	2.0
2	E	76	ASP	2.0
4	G	173	ASP	2.0
3	C	4	LYS	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 [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($\text{\AA}^2$)	Q<0.9
5	GOL	G	965	6/6	0.69	0.26	54,54,56,56	0
5	GOL	H	964	6/6	0.70	0.26	55,55,56,60	0
5	GOL	E	960	6/6	0.77	0.22	61,62,62,63	0
5	GOL	B	966	6/6	0.82	0.16	34,37,41,46	0
5	GOL	E	962	6/6	0.83	0.21	50,51,51,52	0
5	GOL	D	961	6/6	0.85	0.20	51,56,57,59	0
5	GOL	A	968	6/6	0.86	0.14	34,41,44,48	0
5	GOL	B	969	6/6	0.86	0.23	63,64,64,64	0
5	GOL	G	967	6/6	0.87	0.22	55,56,58,58	0
5	GOL	E	963	6/6	0.90	0.13	37,41,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.