



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:25 PM UTC

PDB ID : 5D2N / pdb_00005d2n
Title : Crystal structure of C25-NLV-HLA-A2 complex
Authors : Mariuzza, R.A.; Yang, X.
Deposited on : 2015-08-05
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

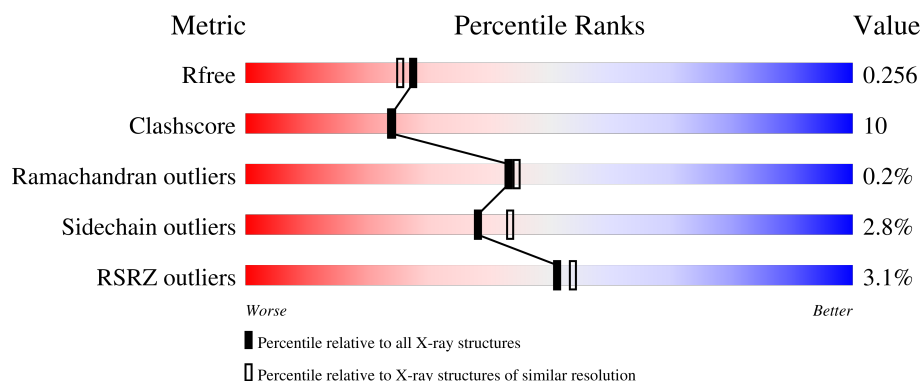
1 Overall quality at a glance

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.



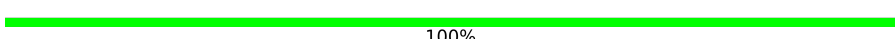
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	C	203	8% 68% 25% ..
1	D	203	6% 75% 21% ..
2	E	247	2% 77% 20% ..
2	F	247	% 82% 17%
3	A	276	2% 77% 21% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	276	 2% 75% 22% ..
4	B	100	 3% 69% 29% •
4	L	100	 % 84% 15% •
5	G	9	 100%
5	I	9	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14050 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 C25 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	198	Total	C	N	O	S	0	0	0
			1554	958	270	316	10			
1	D	198	Total	C	N	O	S	0	0	0
			1554	958	270	316	10			

- Molecule 2 is a protein called C25 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	246	Total	C	N	O	S	0	0	0
			1950	1222	345	377	6			
2	E	245	Total	C	N	O	S	0	0	0
			1942	1218	344	374	6			

- Molecule 3 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	273	Total	C	N	O	S	0	0	0
			2233	1396	407	421	9			
3	A	273	Total	C	N	O	S	0	0	0
			2233	1396	407	421	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	0	MET	-	initiating methionine	UNP P01892
A	0	MET	-	initiating methionine	UNP P01892

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

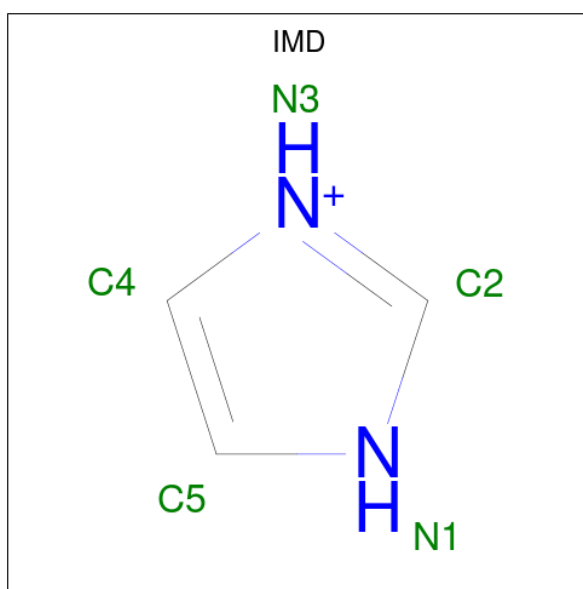
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	initiating methionine	UNP P61769
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 5 is a protein called ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	9	Total	C	N	O	S	0	0	0
			65	42	10	12	1			
5	I	9	Total	C	N	O	S	0	0	0
			65	42	10	12	1			

- Molecule 6 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 7 is water.

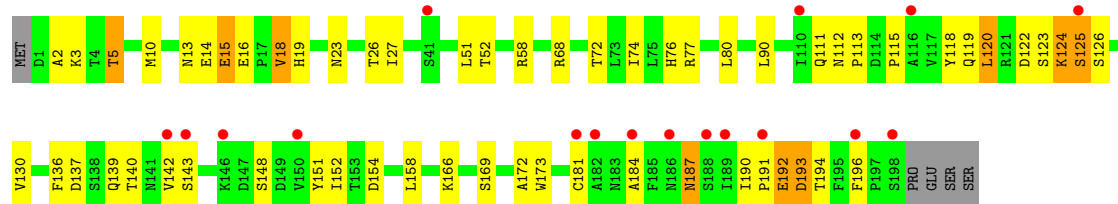
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	54	Total 54	O 54	0	0
7	F	146	Total 146	O 146	0	0
7	H	111	Total 111	O 111	0	0
7	L	71	Total 71	O 71	0	0
7	D	83	Total 83	O 83	0	0
7	E	148	Total 148	O 148	0	0
7	A	117	Total 117	O 117	0	0
7	B	30	Total 30	O 30	0	0
7	G	3	Total 3	O 3	0	0
7	I	3	Total 3	O 3	0	0

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.

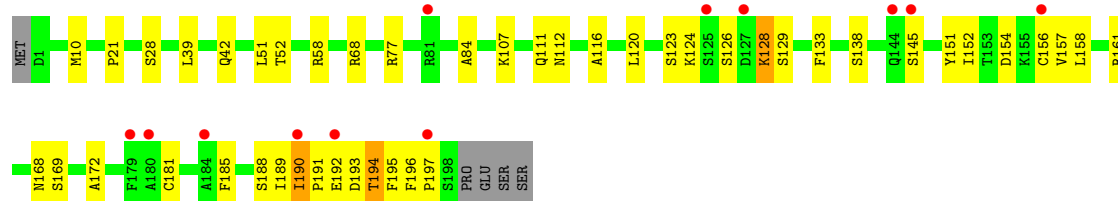
• Molecule 1: C25 alpha

Chain C: 



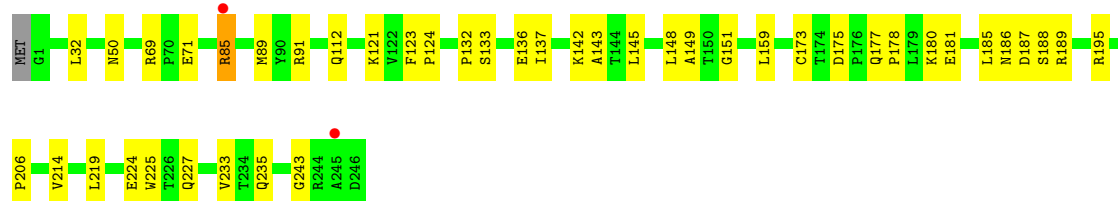
• Molecule 1: C25 alpha

Chain D: 



• Molecule 2: C25 beta

Chain F: 



• Molecule 2: C25 beta

Chain E: 



There are no outlier residues recorded for this chain.

- Molecule 5: ASN-LEU-VAL-PRO-MET-VAL-ALA-THR-VAL

Chain I:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.31Å 124.87Å 193.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.70 – 2.10 40.70 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.70-2.10) 99.2 (40.70-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.204 , 0.253 0.210 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14050	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: IMD

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	C	0.67	0/1587	0.90	4/2157 (0.2%)
1	D	0.80	0/1587	0.94	8/2157 (0.4%)
2	E	0.89	5/1993 (0.3%)	0.96	14/2710 (0.5%)
2	F	0.66	0/2001	0.89	9/2721 (0.3%)
3	A	0.60	0/2298	0.83	3/3120 (0.1%)
3	H	0.74	0/2298	0.91	6/3120 (0.2%)
4	B	0.57	0/859	0.75	1/1162 (0.1%)
4	L	0.64	0/860	0.86	3/1162 (0.3%)
5	G	0.68	0/65	0.72	0/88
5	I	0.63	0/65	0.67	0/88
All	All	0.72	5/13613 (0.0%)	0.89	48/18485 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	91	ARG	C-N	15.33	1.55	1.33
2	E	24	ASP	C-O	-5.93	1.19	1.25
2	E	93	ALA	N-CA	-5.42	1.39	1.45
2	E	179	LEU	C-O	-5.17	1.17	1.24
2	E	48	TYR	C-O	-5.02	1.18	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	91	ARG	O-C-N	-10.80	110.45	123.30
4	L	6	LYS	N-CA-C	-8.91	96.15	110.32
1	D	124	LYS	N-CA-C	-7.98	96.22	109.46
1	C	181	CYS	N-CA-C	7.65	120.59	111.33
2	E	126	GLU	N-CA-C	-7.08	98.19	109.59
2	E	124	PRO	CA-C-N	-6.87	113.58	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	124	PRO	C-N-CA	-6.87	113.58	120.31
3	H	56	GLY	CA-C-N	6.34	126.26	119.28
3	H	56	GLY	C-N-CA	6.34	126.26	119.28
1	D	128	LYS	N-CA-C	6.33	120.59	109.96
2	F	50	ASN	N-CA-C	-6.25	98.08	108.34
3	H	222	GLU	N-CA-C	6.23	119.62	109.59
1	C	193	ASP	N-CA-C	-6.21	104.28	113.72
2	F	124	PRO	CA-C-N	-5.96	114.17	120.66
2	F	124	PRO	C-N-CA	-5.96	114.17	120.66
2	F	123	PHE	CA-C-N	-5.88	114.33	120.38
2	F	123	PHE	C-N-CA	-5.88	114.33	120.38
2	E	22	ARG	N-CA-C	5.82	118.96	109.59
3	H	267	PRO	N-CA-C	-5.78	105.49	113.53
2	E	182	GLN	CA-C-N	5.73	126.11	119.47
2	E	182	GLN	C-N-CA	5.73	126.11	119.47
2	E	24	ASP	CA-C-N	-5.69	114.89	120.52
2	E	24	ASP	C-N-CA	-5.69	114.89	120.52
2	E	110	GLY	N-CA-C	5.67	118.64	112.29
1	C	196	PHE	CA-C-N	5.64	126.89	119.84
1	C	196	PHE	C-N-CA	5.64	126.89	119.84
1	D	154	ASP	N-CA-C	-5.54	103.59	110.41
2	E	50	ASN	N-CA-C	-5.51	99.31	108.34
2	E	93	ALA	N-CA-C	-5.50	100.94	109.24
1	D	196	PHE	CA-C-N	-5.46	114.97	120.21
1	D	196	PHE	C-N-CA	-5.46	114.97	120.21
1	D	112	ASN	CA-C-N	-5.41	114.67	120.03
1	D	112	ASN	C-N-CA	-5.41	114.67	120.03
3	A	56	GLY	CA-C-N	5.36	125.18	119.28
3	A	56	GLY	C-N-CA	5.36	125.18	119.28
2	E	69	ARG	CA-C-N	5.34	125.01	119.56
2	E	69	ARG	C-N-CA	5.34	125.01	119.56
4	L	4	THR	CA-C-N	-5.25	114.51	119.76
4	L	4	THR	C-N-CA	-5.25	114.51	119.76
3	H	17	ARG	N-CA-C	5.18	121.83	110.80
2	F	69	ARG	CA-C-N	5.14	125.18	119.32
2	F	69	ARG	C-N-CA	5.14	125.18	119.32
2	F	175	ASP	CA-C-N	5.11	124.61	119.19
2	F	175	ASP	C-N-CA	5.11	124.61	119.19
3	H	28	VAL	N-CA-C	-5.10	100.31	107.75
4	B	67	TYR	N-CA-C	5.08	116.97	108.99
1	D	190	ILE	N-CA-C	5.06	113.72	109.02
3	A	28	VAL	N-CA-C	-5.02	100.42	107.75

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	C	1554	0	1470	51	1
1	D	1554	0	1470	29	0
2	E	1942	0	1852	37	0
2	F	1950	0	1856	30	0
3	A	2233	0	2084	46	1
3	H	2233	0	2084	47	0
4	B	836	0	803	22	0
4	L	837	0	803	12	0
5	G	65	0	74	0	0
5	I	65	0	74	0	0
6	A	10	0	10	2	0
6	C	5	0	5	2	0
7	A	117	0	0	5	0
7	B	30	0	0	0	0
7	C	54	0	0	2	0
7	D	83	0	0	3	1
7	E	148	0	0	2	0
7	F	146	0	0	4	0
7	G	3	0	0	0	0
7	H	111	0	0	2	1
7	I	3	0	0	0	0
7	L	71	0	0	0	0
All	All	14050	0	12585	258	2

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 10.

All (258) 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)
3:A:111:ARG:HD2	3:A:113:TYR:OH	1.22	1.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:THR:HG22	1:C:68:ARG:HD3	1.30	1.10
3:A:111:ARG:CD	3:A:113:TYR:OH	2.09	1.01
4:L:3:ARG:HH21	4:L:3:ARG:HG2	1.28	0.97
1:C:124:LYS:O	1:C:126:SER:N	1.96	0.96
3:A:266:LEU:HD13	3:A:270:LEU:HD13	1.46	0.94
3:A:108:ARG:HH21	3:A:108:ARG:HG3	1.35	0.92
2:F:177:GLN:HG3	2:F:178:PRO:HD2	1.52	0.90
1:D:188:SER:O	1:D:189:ILE:HD13	1.74	0.88
1:C:51:LEU:O	1:C:68:ARG:NH1	2.09	0.86
3:A:255:GLN:NE2	3:A:274:TRP:O	2.09	0.85
3:A:111:ARG:HD2	3:A:113:TYR:CZ	2.11	0.85
1:D:52:THR:HG22	1:D:68:ARG:HD3	1.58	0.83
1:D:156:CYS:C	2:E:173:CYS:SG	2.62	0.82
3:A:103:VAL:CG1	3:A:165:VAL:HG23	2.11	0.81
1:D:188:SER:C	1:D:189:ILE:HD13	2.07	0.80
3:H:220:ASP:OD2	3:H:256:ARG:NH1	2.14	0.80
2:E:175:ASP:OD1	2:E:195:ARG:NH2	2.14	0.80
1:C:52:THR:HG22	1:C:68:ARG:CD	2.12	0.78
2:E:49:PHE:CE2	2:E:54:GLN:HG3	2.21	0.76
3:A:65:ARG:NH2	7:A:403:HOH:O	2.19	0.75
3:H:103:VAL:CG1	3:H:165:VAL:HG23	2.17	0.73
1:C:148:SER:O	7:C:401:HOH:O	2.06	0.72
3:A:108:ARG:HH21	3:A:108:ARG:CG	2.03	0.71
2:F:85:ARG:HD2	2:F:85:ARG:O	1.91	0.71
2:F:180:LYS:HE2	2:F:188:SER:HB3	1.73	0.70
3:H:178:THR:HA	3:H:181:ARG:HD3	1.72	0.70
4:L:3:ARG:HG2	4:L:3:ARG:NH2	2.02	0.70
3:H:220:ASP:CG	3:H:256:ARG:HE	2.00	0.70
4:L:5:PRO:HB3	4:L:27:VAL:CG2	2.22	0.70
3:H:6:ARG:NE	3:H:113:TYR:OH	2.24	0.69
2:E:151:GLY:O	2:E:189:ARG:HD2	1.91	0.69
1:C:124:LYS:NZ	4:B:89:GLN:OE1	2.24	0.69
3:A:111:ARG:CD	3:A:113:TYR:CZ	2.73	0.68
4:B:22:PHE:CZ	4:B:69:GLU:HG3	2.27	0.68
2:F:181:GLU:OE2	7:F:301:HOH:O	2.11	0.68
4:B:22:PHE:CE1	4:B:69:GLU:HG3	2.29	0.67
4:L:3:ARG:HH21	4:L:3:ARG:CG	2.05	0.67
3:A:91:GLY:N	7:A:401:HOH:O	2.13	0.67
4:B:4:THR:HG22	4:B:5:PRO:HD2	1.78	0.65
3:A:271:THR:C	3:A:272:LEU:HD23	2.22	0.65
3:A:91:GLY:CA	7:A:401:HOH:O	2.46	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:103:VAL:HG12	3:A:165:VAL:HG23	1.79	0.64
1:C:152:ILE:HD11	1:C:184:ALA:HB1	1.80	0.64
3:H:21:ARG:NH1	7:H:301:HOH:O	2.31	0.63
4:B:4:THR:HG23	4:B:86:THR:OG1	1.98	0.63
4:B:13:HIS:HB2	4:B:21:ASN:HD21	1.62	0.63
3:H:106:ASP:OD2	3:H:108:ARG:HD3	1.98	0.63
1:C:10:MET:HE1	1:C:19:HIS:O	1.99	0.63
4:B:41:LYS:HG3	4:B:78:TYR:CE2	2.34	0.62
1:C:72:THR:HG22	1:C:74:ILE:HD12	1.81	0.62
2:F:121:LYS:NZ	2:F:187:ASP:OD2	2.32	0.62
1:C:118:TYR:CD2	2:F:136:GLU:HB2	2.35	0.62
3:A:49:ALA:O	3:A:52:ILE:HG22	2.01	0.61
3:A:91:GLY:HA3	7:A:401:HOH:O	2.00	0.61
3:H:60:TRP:O	3:H:64:THR:HG22	2.01	0.61
2:F:132:PRO:HG3	2:F:143:ALA:HB1	1.82	0.61
1:C:3:LYS:H	6:C:301:IMD:C2	2.14	0.61
1:C:80:LEU:HD11	1:C:166:LYS:HD3	1.84	0.60
4:B:4:THR:CG2	4:B:5:PRO:HD2	2.32	0.60
2:E:33:TYR:O	2:E:92:CYS:HA	2.02	0.60
1:D:58:ARG:HG2	1:D:58:ARG:HH11	1.66	0.60
2:E:91:ARG:NH2	7:E:301:HOH:O	2.13	0.60
3:H:252:GLY:N	3:H:254:GLU:OE2	2.35	0.60
3:H:165:VAL:HG22	3:H:169:ARG:CZ	2.32	0.59
7:D:343:HOH:O	3:A:65:ARG:HD3	2.01	0.59
2:F:206:PRO:HA	2:F:243:GLY:O	2.02	0.59
1:D:192:GLU:O	1:D:193:ASP:HB2	2.03	0.58
2:E:181:GLU:OE1	7:E:302:HOH:O	2.17	0.58
1:C:122:ASP:OD1	1:C:123:SER:N	2.36	0.58
3:A:129:ASP:O	3:A:131:ARG:NH1	2.36	0.58
3:H:218:GLN:NE2	3:H:221:GLY:HA2	2.19	0.58
1:D:190:ILE:HG22	1:D:191:PRO:O	2.03	0.58
1:C:112:ASN:N	1:C:113:PRO:HD3	2.19	0.58
2:F:180:LYS:NZ	2:F:186:ASN:HA	2.17	0.58
1:D:157:VAL:N	2:E:173:CYS:SG	2.76	0.57
3:H:22:PHE:CD2	3:H:71:SER:HB3	2.40	0.57
1:C:58:ARG:HE	1:C:58:ARG:HA	1.68	0.56
1:C:58:ARG:HA	1:C:58:ARG:NE	2.20	0.56
2:F:159:LEU:HD23	2:F:159:LEU:C	2.29	0.56
2:F:227:GLN:NE2	7:F:304:HOH:O	2.39	0.56
1:D:126:SER:OG	1:D:128:LYS:HB2	2.06	0.56
3:H:226:GLN:O	3:H:227:ASP:HB2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ASN:O	1:C:16:GLU:HG2	2.06	0.56
2:E:122:VAL:HG21	2:E:219:LEU:HD21	1.88	0.56
1:D:28:SER:O	1:D:68:ARG:NH2	2.39	0.55
1:C:118:TYR:CZ	2:F:136:GLU:HA	2.42	0.55
3:A:117:ALA:HB2	4:B:60:TRP:CE2	2.41	0.55
3:H:44:ARG:NH1	3:H:64:THR:HG21	2.22	0.55
3:A:272:LEU:HD23	3:A:272:LEU:N	2.22	0.55
2:E:180:LYS:NZ	2:E:185:LEU:O	2.39	0.55
4:B:17:ASN:OD1	4:B:97:ARG:NH1	2.40	0.55
3:H:103:VAL:HG11	3:H:165:VAL:HG23	1.89	0.54
3:H:218:GLN:HE21	3:H:221:GLY:HA2	1.71	0.54
4:B:13:HIS:CB	4:B:21:ASN:HD21	2.21	0.54
1:C:111:GLN:O	1:C:112:ASN:HB2	2.08	0.54
3:A:184:ALA:HB2	3:A:265:GLY:O	2.08	0.54
1:D:185:PHE:HB3	1:D:190:ILE:HD11	1.90	0.53
1:C:118:TYR:CE2	2:F:136:GLU:HB2	2.43	0.53
3:H:249:VAL:HG12	3:H:257:TYR:CZ	2.44	0.53
3:A:123:TYR:CZ	3:A:140:ALA:HA	2.44	0.53
1:C:115:PRO:O	1:C:194:THR:HA	2.09	0.53
3:H:249:VAL:HG12	3:H:257:TYR:CE2	2.44	0.53
1:D:158:LEU:HB3	2:E:173:CYS:HB2	1.91	0.53
2:E:49:PHE:CZ	2:E:54:GLN:HG3	2.43	0.52
1:C:27:ILE:HG21	1:C:68:ARG:O	2.10	0.52
2:F:133:SER:O	2:F:137:ILE:HG13	2.10	0.52
1:D:120:LEU:O	1:D:129:SER:HB2	2.10	0.52
1:C:192:GLU:O	1:C:193:ASP:HB3	2.10	0.51
1:D:52:THR:HG22	1:D:68:ARG:CD	2.35	0.51
1:D:181:CYS:N	7:D:302:HOH:O	2.05	0.51
3:A:30:ASP:OD1	6:A:301:IMD:H5	2.11	0.51
1:C:10:MET:HE2	1:C:18:VAL:HG12	1.92	0.51
1:D:169:SER:OG	2:E:195:ARG:HD3	2.10	0.51
2:E:89:MET:HE1	2:E:112:GLN:HB2	1.91	0.51
2:E:93:ALA:HA	2:E:106:PHE:O	2.10	0.51
3:H:127:LYS:HE2	3:H:134:THR:OG1	2.10	0.51
3:A:35:ARG:HG2	3:A:48:ARG:HD3	1.93	0.51
1:C:10:MET:HE2	1:C:18:VAL:CG1	2.41	0.51
2:F:180:LYS:HE3	7:F:328:HOH:O	2.10	0.51
3:H:177:GLU:HB3	7:H:326:HOH:O	2.11	0.51
3:H:127:LYS:HD3	3:H:132:SER:OG	2.11	0.50
3:H:117:ALA:HB2	4:L:60:TRP:CE2	2.47	0.50
1:C:137:ASP:OD2	1:C:139:GLN:NE2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:VAL:HG22	2:E:79:ILE:HB	1.94	0.50
1:C:169:SER:HB3	7:C:406:HOH:O	2.11	0.50
1:C:158:LEU:HB3	2:F:173:CYS:HB2	1.94	0.49
3:A:117:ALA:HB2	4:B:60:TRP:CD2	2.47	0.49
1:D:116:ALA:HA	1:D:195:PHE:O	2.12	0.49
1:D:151:TYR:O	1:D:172:ALA:HA	2.11	0.49
1:C:192:GLU:C	1:C:194:THR:H	2.19	0.49
3:H:106:ASP:OD2	3:H:108:ARG:CD	2.60	0.49
3:A:11:SER:HA	3:A:21:ARG:O	2.12	0.49
2:E:19:VAL:HG13	2:E:82:THR:HG21	1.95	0.49
2:E:132:PRO:HD2	2:E:203:TRP:CZ2	2.48	0.49
1:C:14:GLU:OE1	1:C:166:LYS:NZ	2.34	0.49
3:A:108:ARG:CG	3:A:108:ARG:NH2	2.70	0.49
3:A:215:LEU:CD2	3:A:261:VAL:HG22	2.43	0.49
4:B:13:HIS:HB2	4:B:21:ASN:ND2	2.27	0.49
1:C:26:THR:O	1:C:26:THR:OG1	2.29	0.49
1:C:124:LYS:C	1:C:126:SER:N	2.68	0.49
3:H:162:GLY:O	3:H:166:GLU:HG3	2.13	0.49
3:A:105:SER:C	3:A:107:TRP:H	2.21	0.48
2:F:85:ARG:HD2	2:F:85:ARG:C	2.37	0.48
3:H:49:ALA:O	3:H:52:ILE:HG22	2.14	0.48
3:H:218:GLN:HG2	3:H:222:GLU:C	2.39	0.48
4:B:81:ARG:HG3	4:B:92:ILE:HG12	1.96	0.48
1:D:39:LEU:HD23	1:D:84:ALA:HB2	1.96	0.48
2:E:19:VAL:HG13	2:E:82:THR:CG2	2.44	0.47
4:B:1:ILE:O	4:B:1:ILE:HD12	2.14	0.47
1:D:10:MET:HE1	1:D:21:PRO:CD	2.44	0.47
3:H:218:GLN:NE2	3:H:221:GLY:C	2.72	0.47
3:H:271:THR:O	3:H:272:LEU:HD23	2.14	0.47
2:E:159:LEU:C	2:E:159:LEU:HD23	2.39	0.47
4:B:20:SER:HA	4:B:71:THR:HG22	1.95	0.47
1:C:3:LYS:CG	1:C:90:LEU:HD23	2.45	0.47
1:C:5:THR:HG22	1:C:23:ASN:OD1	2.15	0.47
1:C:136:PHE:CD2	1:C:140:THR:HB	2.50	0.47
4:L:5:PRO:HB3	4:L:27:VAL:HG23	1.95	0.47
1:C:2:ALA:HA	6:C:301:IMD:H2	1.97	0.46
2:E:13:THR:HG21	2:E:19:VAL:CG1	2.45	0.46
3:H:219:ARG:O	3:H:220:ASP:C	2.55	0.46
1:D:51:LEU:O	1:D:68:ARG:NH1	2.42	0.46
3:A:102:ASP:OD2	3:A:113:TYR:OH	2.28	0.46
3:A:32:GLN:NE2	4:B:53:ASP:OD2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:21:ARG:HD3	3:H:39:ASP:OD2	2.16	0.46
2:E:123:PHE:CD1	2:E:189:ARG:HD3	2.51	0.45
3:H:131:ARG:HH22	3:H:157:ARG:NH2	2.14	0.45
1:C:192:GLU:C	1:C:194:THR:N	2.73	0.45
3:A:268:LYS:HB2	3:A:269:PRO:HD2	1.97	0.45
3:H:11:SER:HA	3:H:21:ARG:O	2.16	0.45
2:E:13:THR:HG21	2:E:82:THR:HG21	1.99	0.45
1:C:3:LYS:HG3	1:C:90:LEU:HD23	1.97	0.45
3:A:230:LEU:CD1	3:A:245:ALA:HB2	2.47	0.45
3:H:31:THR:OG1	3:H:209:TYR:OH	2.32	0.45
3:H:217:TRP:CE2	3:H:247:VAL:HG12	2.51	0.45
4:L:51:HIS:HA	4:L:65:LEU:O	2.17	0.45
2:E:89:MET:CE	2:E:112:GLN:HB2	2.47	0.45
3:H:182:THR:HG21	3:H:264:GLU:HG2	1.98	0.44
4:L:21:ASN:OD1	4:L:22:PHE:N	2.45	0.44
1:C:74:ILE:HD12	1:C:74:ILE:N	2.32	0.44
3:H:218:GLN:HE21	3:H:221:GLY:CA	2.30	0.44
3:H:219:ARG:O	3:H:220:ASP:HB2	2.18	0.44
1:D:190:ILE:HG23	1:D:194:THR:OG1	2.17	0.44
1:C:15:GLU:CD	1:C:77:ARG:HE	2.26	0.44
2:E:161:TRP:HB2	2:E:168:VAL:HG22	1.98	0.44
3:H:202:ARG:HD2	3:H:244:TRP:CD2	2.52	0.44
2:E:175:ASP:HB2	2:E:192:LEU:HD12	1.99	0.44
2:F:185:LEU:C	2:F:187:ASP:H	2.25	0.44
4:L:51:HIS:HB3	4:L:66:TYR:CD2	2.53	0.44
3:A:8:PHE:CZ	6:A:301:IMD:H2	2.53	0.44
2:F:151:GLY:O	2:F:189:ARG:HD2	2.17	0.44
3:A:108:ARG:HG3	3:A:108:ARG:NH2	2.16	0.44
1:C:72:THR:HG22	1:C:74:ILE:CD1	2.47	0.44
3:A:5:MET:HB2	3:A:168:LEU:HD13	2.00	0.44
3:H:15:PRO:HG2	3:H:90:ALA:O	2.18	0.43
1:D:145:SER:OG	1:D:152:ILE:HG13	2.17	0.43
1:D:195:PHE:CE1	1:D:197:PRO:HD3	2.53	0.43
1:C:112:ASN:N	1:C:113:PRO:CD	2.81	0.43
2:E:22:ARG:HG2	2:E:23:CYS:N	2.33	0.43
2:F:180:LYS:HZ3	2:F:186:ASN:HA	1.81	0.43
2:E:17:GLN:O	2:E:82:THR:HG23	2.18	0.43
2:F:89:MET:HE1	2:F:112:GLN:HB2	2.01	0.43
2:F:186:ASN:HB2	7:F:411:HOH:O	2.18	0.43
1:D:133:PHE:O	1:D:169:SER:HA	2.19	0.43
3:A:50:PRO:HA	3:A:53:GLU:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LEU:N	1:C:120:LEU:HD12	2.33	0.43
2:E:1:GLY:HA3	2:E:27:SER:OG	2.18	0.43
2:F:145:LEU:HD12	2:F:145:LEU:H	1.83	0.43
2:E:62:ASN:OD1	2:E:64:ARG:HB2	2.19	0.42
2:E:151:GLY:C	2:E:189:ARG:HD2	2.43	0.42
2:F:32:LEU:C	2:F:32:LEU:HD23	2.44	0.42
3:A:257:TYR:OH	7:A:404:HOH:O	2.21	0.42
3:A:120:GLY:O	4:B:1:ILE:HD11	2.18	0.42
2:E:125:PRO:HD3	2:E:216:PHE:HB2	2.01	0.42
4:B:16:GLU:OE2	4:B:19:LYS:HD2	2.20	0.42
4:B:29:GLY:HA2	4:B:61:SER:OG	2.18	0.42
1:C:130:VAL:HG12	1:C:173:TRP:HB3	2.02	0.42
2:F:89:MET:HG2	2:F:91:ARG:CZ	2.50	0.42
3:H:202:ARG:HD3	3:H:244:TRP:CE3	2.54	0.42
2:F:224:GLU:OE1	2:F:224:GLU:HA	2.20	0.42
3:H:89:GLU:OE1	2:E:5:SER:OG	2.36	0.42
4:L:37:VAL:HG22	4:L:82:VAL:HG22	2.01	0.42
3:A:28:VAL:O	3:A:29:ASP:C	2.62	0.42
1:C:152:ILE:CD1	1:C:184:ALA:HB1	2.49	0.41
1:D:77:ARG:HD3	7:D:372:HOH:O	2.19	0.41
1:D:107:LYS:HB3	1:D:138:SER:HB3	2.02	0.41
1:C:151:TYR:O	1:C:172:ALA:HA	2.20	0.41
3:H:215:LEU:HD22	3:H:261:VAL:HG22	2.02	0.41
1:D:123:SER:HB2	2:E:131:GLU:HG3	2.02	0.41
4:L:5:PRO:CB	4:L:27:VAL:HG23	2.51	0.41
1:D:157:VAL:HG22	1:D:168:ASN:OD1	2.21	0.41
1:C:190:ILE:HD12	1:C:194:THR:HG21	2.02	0.41
2:E:163:VAL:CG2	2:E:168:VAL:HG11	2.50	0.41
3:A:22:PHE:CD1	3:A:71:SER:HB3	2.56	0.41
2:F:225:TRP:CZ2	2:F:227:GLN:HB2	2.54	0.41
1:C:142:VAL:HG12	1:C:143:SER:N	2.36	0.41
1:C:125:SER:O	1:C:125:SER:OG	2.23	0.41
2:F:149:ALA:HB2	2:F:214:VAL:HG21	2.03	0.41
3:A:28:VAL:HG11	3:A:179:LEU:HD13	2.02	0.41
3:A:42:SER:O	3:A:44:ARG:HG2	2.21	0.41
3:A:207:SER:HA	3:A:240:THR:HB	2.02	0.41
1:C:119:GLN:C	1:C:120:LEU:HD12	2.46	0.41
4:L:7:ILE:HD12	4:L:91:LYS:HD2	2.02	0.41
3:H:137:ASP:O	3:H:141:GLN:HG2	2.20	0.41
3:H:185:PRO:HA	3:H:208:PHE:HB3	2.03	0.41
2:E:229:ARG:HH11	2:E:229:ARG:HD3	1.70	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:39:LEU:HD12	4:B:68:THR:HG22	2.03	0.41
1:C:76:HIS:C	1:C:77:ARG:HG2	2.46	0.40
3:A:7:TYR:HB3	3:A:9:PHE:CZ	2.56	0.40
2:F:233:VAL:O	2:F:235:GLN:HG2	2.21	0.40
3:H:220:ASP:OD2	3:H:256:ARG:NE	2.52	0.40
4:B:33:SER:HB3	4:B:62:PHE:CE2	2.56	0.40
2:F:136:GLU:HG2	2:F:142:LYS:O	2.21	0.40
3:H:187:THR:OG1	3:H:272:LEU:HD11	2.22	0.40
3:H:257:TYR:CD1	3:H:257:TYR:N	2.89	0.40
2:E:163:VAL:HA	2:E:209:HIS:O	2.22	0.40
3:A:82:ARG:HD2	3:A:89:GLU:HA	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ASN:O	3:A:268:LYS:NZ[1_455]	2.07	0.13
7:H:341:HOH:O	7:D:381:HOH:O[1_455]	2.12	0.08

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	C	196/203 (97%)	182 (93%)	12 (6%)	2 (1%)	12	9
1	D	196/203 (97%)	185 (94%)	11 (6%)	0	100	100
2	E	243/247 (98%)	235 (97%)	8 (3%)	0	100	100
2	F	244/247 (99%)	238 (98%)	6 (2%)	0	100	100
3	A	271/276 (98%)	263 (97%)	8 (3%)	0	100	100
3	H	271/276 (98%)	262 (97%)	8 (3%)	1 (0%)	30	28
4	B	98/100 (98%)	93 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
5	G	7/9 (78%)	7 (100%)	0	0	100	100
5	I	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1631/1670 (98%)	1568 (96%)	60 (4%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	125	SER
1	C	191	PRO
3	H	15	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	C	179/184 (97%)	171 (96%)	8 (4%)	24	25
1	D	179/184 (97%)	175 (98%)	4 (2%)	45	53
2	E	210/212 (99%)	205 (98%)	5 (2%)	43	49
2	F	211/212 (100%)	206 (98%)	5 (2%)	43	49
3	A	230/232 (99%)	224 (97%)	6 (3%)	40	46
3	H	230/232 (99%)	224 (97%)	6 (3%)	40	46
4	B	95/95 (100%)	90 (95%)	5 (5%)	20	19
4	L	95/95 (100%)	93 (98%)	2 (2%)	47	54
5	G	8/8 (100%)	8 (100%)	0	100	100
5	I	8/8 (100%)	8 (100%)	0	100	100
All	All	1445/1462 (99%)	1404 (97%)	41 (3%)	38	43

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

Mol	Chain	Res	Type
1	C	5	THR
1	C	15	GLU
1	C	18	VAL
1	C	120	LEU
1	C	124	LYS
1	C	154	ASP
1	C	187	ASN
1	C	192	GLU
2	F	71	GLU
2	F	85	ARG
2	F	148	LEU
2	F	195	ARG
2	F	219	LEU
3	H	15	PRO
3	H	35	ARG
3	H	108	ARG
3	H	224	GLN
3	H	247	VAL
3	H	254	GLU
4	L	3	ARG
4	L	19	LYS
1	D	42	GLN
1	D	111	GLN
1	D	161	ARG
1	D	194	THR
2	E	19	VAL
2	E	91	ARG
2	E	109	SER
2	E	166	LYS
2	E	195	ARG
3	A	48	ARG
3	A	108	ARG
3	A	138	MET
3	A	223	ASP
3	A	254	GLU
3	A	272	LEU
4	B	1	ILE
4	B	44	GLU
4	B	69	GLU
4	B	70	PHE
4	B	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	ASN
2	F	222	ASN
3	H	96	GLN
3	H	218	GLN
1	D	23	ASN
1	D	187	ASN
2	E	54	GLN
2	E	182	GLN
3	A	54	GLN
3	A	96	GLN
3	A	141	GLN
3	A	145	HIS
3	A	180	GLN
3	A	224	GLN

5.3.3 RNA [i](#)

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](#)

3 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	$\# Z > 2$
6	IMD	C	301	-	5,5,5	0.62	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	IMD	A	302	-	5,5,5	0.53	0	5,5,5	0.38	0
6	IMD	A	301	-	5,5,5	0.48	0	5,5,5	0.55	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	IMD	C	301	-	-	-	0/1/1/1
6	IMD	A	302	-	-	-	0/1/1/1
6	IMD	A	301	-	-	-	0/1/1/1

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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	301	IMD	2	0
6	A	301	IMD	2	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	C	198/203 (97%)	0.65	17 (8%) 16 17	28, 48, 77, 83	0
1	D	198/203 (97%)	0.39	12 (6%) 27 29	26, 40, 66, 77	0
2	E	245/247 (99%)	0.01	4 (1%) 70 73	26, 35, 51, 63	0
2	F	246/247 (99%)	0.08	2 (0%) 82 84	26, 38, 56, 65	0
3	A	273/276 (98%)	0.26	6 (2%) 62 65	27, 39, 54, 62	2 (0%)
3	H	273/276 (98%)	0.19	6 (2%) 62 65	25, 38, 56, 76	1 (0%)
4	B	100/100 (100%)	0.53	3 (3%) 52 55	29, 45, 74, 77	0
4	L	100/100 (100%)	-0.08	1 (1%) 79 81	27, 35, 52, 59	2 (2%)
5	G	9/9 (100%)	-0.54	0 100 100	26, 27, 29, 33	0
5	I	9/9 (100%)	-0.45	0 100 100	25, 27, 29, 33	0
All	All	1651/1670 (98%)	0.23	51 (3%) 51 54	25, 39, 63, 83	5 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	156	CYS	3.8
3	H	104	GLY	3.6
2	E	1	GLY	3.4
3	H	221	GLY	3.2
1	C	189	ILE	3.0
1	C	188	SER	2.9
1	D	125	SER	2.9
1	D	145	SER	2.8
4	B	1	ILE	2.7
2	F	245	ALA	2.7
4	B	71	THR	2.6
2	E	179	LEU	2.6
1	C	198	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	142	VAL	2.6
1	C	125	SER	2.5
1	C	184	ALA	2.5
1	C	110	ILE	2.5
1	C	143	SER	2.4
3	A	270	LEU	2.4
3	H	105	SER	2.4
1	C	181	CYS	2.4
3	A	51	TRP	2.4
1	D	180	ALA	2.3
3	H	136	ALA	2.3
3	A	2	SER	2.3
1	C	116	ALA	2.3
1	C	182	ALA	2.3
1	D	184	ALA	2.3
1	D	197	PRO	2.2
1	C	191	PRO	2.2
2	E	245	ALA	2.2
3	H	107	TRP	2.2
1	C	196	PHE	2.2
1	D	179	PHE	2.2
1	C	41	SER	2.2
3	A	181	ARG	2.2
3	A	113	TYR	2.2
1	D	127	ASP	2.2
1	D	192	GLU	2.1
1	C	186	ASN	2.1
1	D	144	GLN	2.1
1	D	190	ILE	2.1
2	F	85	ARG	2.1
1	D	81	ARG	2.1
3	H	181	ARG	2.1
3	A	107	TRP	2.1
4	B	78	TYR	2.1
2	E	201	THR	2.0
1	C	146	LYS	2.0
1	C	150	VAL	2.0
4	L	69	GLU	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
6	IMD	A	301	5/5	0.73	0.18	49,50,54,55	0
6	IMD	C	301	5/5	0.78	0.15	45,46,50,51	0
6	IMD	A	302	5/5	0.79	0.25	43,48,49,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.