



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 10:11 pm GMT

PDB ID : 6SS7
Title : Human Leukocyte Antigen Class I A02 Carrying LLWAGPMAV
Authors : Rizkallah, P.J.; Bovay, A.
Deposited on : 2019-09-06
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

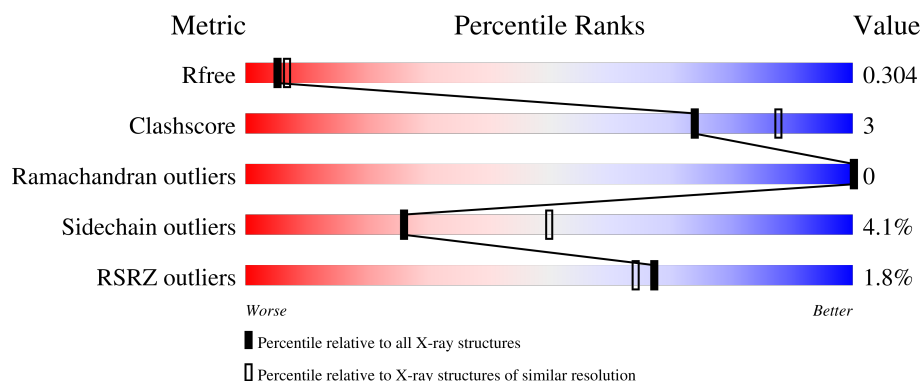
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>
1	D	276	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>
2	B	100	<div> <div>%</div> <div>88%</div> <div>11%</div> </div>
2	E	100	<div> <div>3%</div> <div>85%</div> <div>13%</div> </div>
3	C	9	<div> <div>56%</div> <div>44%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	9	 67% 33%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6717 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 I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	D	276	Total	C	N	O	S	0	1	0
			2261	1413	411	428	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
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called LEU-LEU-TRP-ALA-GLY-PRO-MET-ALA-VAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			67	46	10	10	1			
3	F	9	Total	C	N	O	S	0	0	0
			67	46	10	10	1			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

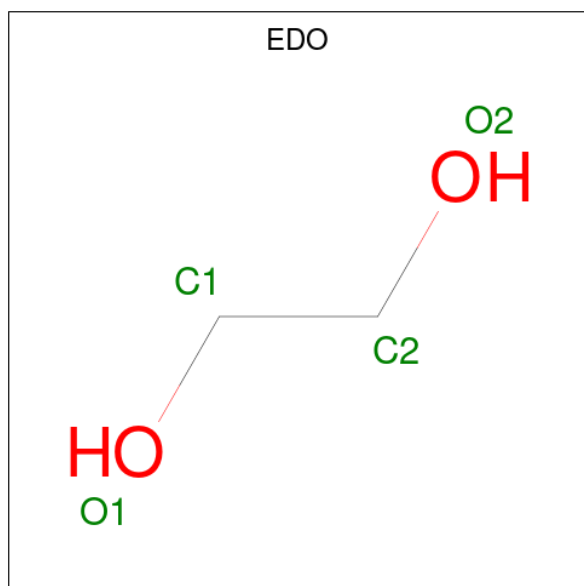
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

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



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	87	Total	O	0	0
			87	87		
8	B	58	Total	O	0	0
			58	58		
8	C	4	Total	O	0	0
			4	4		
8	D	85	Total	O	0	0
			85	85		
8	E	38	Total	O	0	0
			38	38		

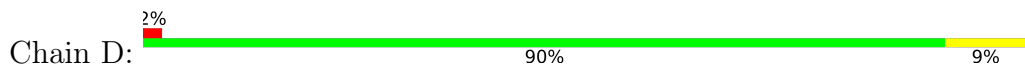
3 Residue-property plots [i](#)

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.

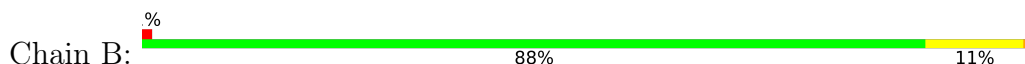
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



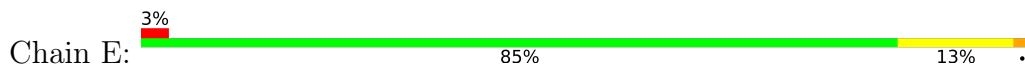
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: LEU-LEU-TRP-ALA-GLY-PRO-MET-ALA-VAL



- Molecule 3: LEU-LEU-TRP-ALA-GLY-PRO-MET-ALA-VAL

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.56Å 169.25Å 49.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.62 – 2.50 84.62 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (84.62-2.50) 99.5 (84.62-2.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.37Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.226 , 0.304 0.229 , 0.304	Depositor DCC
R_{free} test set	1757 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtrriage
Anisotropy	0.538	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6717	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 30.68 % 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 1.2558e-03. 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: NA, EDO, SO4, 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	0.91	1/2320 (0.0%)	0.98	6/3149 (0.2%)
1	D	0.93	0/2327	0.97	4/3159 (0.1%)
2	B	0.97	0/860	1.05	4/1162 (0.3%)
2	E	0.90	0/860	1.02	3/1162 (0.3%)
3	C	1.02	0/69	1.09	0/93
3	F	1.10	0/69	1.17	0/93
All	All	0.93	1/6505 (0.0%)	1.00	17/8818 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLU	CD-OE2	5.87	1.32	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	ASP	CB-CG-OD1	7.20	124.78	118.30
2	B	97	ARG	NE-CZ-NH2	-6.97	116.82	120.30
2	E	34	ASP	CB-CG-OD2	-6.82	112.17	118.30
1	A	129	ASP	CB-CG-OD1	6.62	124.26	118.30
1	D	129	ASP	CB-CG-OD1	6.57	124.21	118.30
2	B	97	ARG	NE-CZ-NH1	6.39	123.50	120.30
2	E	81	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	A	39	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	157	ARG	NE-CZ-NH1	-6.17	117.22	120.30
2	B	81	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	A	65	ARG	NE-CZ-NH2	5.80	123.20	120.30
2	E	81	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	170	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	B	45	ARG	NE-CZ-NH1	5.51	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	35	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	39	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	169	ARG	NE-CZ-NH1	5.17	122.89	120.30

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	12	0
1	D	2261	0	2111	19	0
2	B	837	0	803	5	0
2	E	837	0	803	4	0
3	C	67	0	72	2	0
3	F	67	0	72	2	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	8	0	12	1	0
5	B	12	0	18	0	0
5	D	8	0	12	0	0
6	A	20	0	0	0	0
6	B	5	0	0	0	0
6	D	15	0	0	0	0
6	E	10	0	0	0	0
7	A	18	0	24	0	0
7	B	12	0	16	0	0
7	D	12	0	16	3	0
8	A	87	0	0	1	0
8	B	58	0	0	0	0
8	C	4	0	0	0	0
8	D	85	0	0	2	1
8	E	38	0	0	0	0
All	All	6717	0	6062	37	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 3.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ARG:HD3	8:D:418:HOH:O	1.65	0.94
1:D:17:ARG:NH1	8:D:401:HOH:O	2.08	0.86
1:D:220:ASP:OD1	7:D:308:GOL:O2	2.07	0.71
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.35	0.61
1:A:264:GLU:HG2	8:A:471:HOH:O	2.01	0.60
3:C:5:GLY:N	3:C:6:PRO:HD3	2.18	0.57
1:D:187:THR:HB	1:D:272:LEU:HD11	1.88	0.56
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.44	0.52
1:D:143:THR:HG23	3:F:9:VAL:HA	1.89	0.52
1:A:82:ARG:HB2	5:A:302:EDO:H21	1.93	0.51
1:A:187:THR:HB	1:A:272:LEU:HD11	1.92	0.51
1:D:13:SER:HB3	1:D:78:LEU:HD13	1.92	0.51
1:A:219:ARG:HG2	1:A:257:TYR:CE1	2.47	0.50
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.95	0.48
2:E:31:HIS:ND1	2:E:32:PRO:HA	2.29	0.48
1:D:256:ARG:HA	7:D:308:GOL:H31	1.96	0.48
1:D:35:ARG:HG2	2:E:53:ASP:OD2	2.15	0.47
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.49	0.47
1:A:35:ARG:NH1	1:A:46:GLU:OE2	2.48	0.46
1:D:35:ARG:NH1	1:D:46:GLU:OE2	2.49	0.45
1:D:248[A]:VAL:O	1:D:248[A]:VAL:HG12	2.16	0.45
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.99	0.45
1:D:74:HIS:CE1	1:D:97:ARG:HH11	2.34	0.45
1:A:219:ARG:CG	1:A:257:TYR:CE1	3.00	0.44
1:D:256:ARG:HA	7:D:308:GOL:H12	1.99	0.44
3:F:5:GLY:N	3:F:6:PRO:HD3	2.32	0.44
1:A:74:HIS:CE1	1:A:97:ARG:HH11	2.36	0.44
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.53	0.44
2:E:25:CYS:HB2	2:E:39:LEU:HD21	2.01	0.43
2:B:31:HIS:ND1	2:B:32:PRO:HA	2.34	0.43
1:D:219:ARG:HG2	1:D:257:TYR:CE1	2.54	0.42
1:D:174:ASN:HD22	1:D:174:ASN:HA	1.69	0.42
1:D:219:ARG:CG	1:D:257:TYR:CE1	3.03	0.41
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.39	0.41
2:B:38:ASP:OD2	1:D:138:MET:SD	2.80	0.40
1:A:143:THR:HG23	3:C:9:VAL:HA	2.01	0.40
1:A:117:ALA:HB2	2:B:60:TRP:CZ2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:408:HOH:O	8:D:408:HOH:O[2_665]	1.56	0.64

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
1	D	275/276 (100%)	266 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
2	E	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	759/770 (99%)	737 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/232 (100%)	226 (97%)	6 (3%)	41	68
1	D	233/232 (100%)	226 (97%)	7 (3%)	36	63
2	B	95/95 (100%)	91 (96%)	4 (4%)	25	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	95/95 (100%)	86 (90%)	9 (10%)	7	14
3	C	6/6 (100%)	5 (83%)	1 (17%)	2	3
3	F	6/6 (100%)	6 (100%)	0	100	100
All	All	667/666 (100%)	640 (96%)	27 (4%)	26	51

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	35	ARG
1	A	219	ARG
1	A	227	ASP
1	A	268	LYS
1	A	275	GLU
2	B	38	ASP
2	B	48	LYS
2	B	70	PHE
2	B	98	ASP
3	C	7	MET
1	D	11	SER
1	D	35	ARG
1	D	53	GLU
1	D	58	GLU
1	D	219	ARG
1	D	227	ASP
1	D	275	GLU
2	E	32	PRO
2	E	34	ASP
2	E	38	ASP
2	E	70	PHE
2	E	75	LYS
2	E	83	ASN
2	E	89	GLN
2	E	98	ASP
2	E	99	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN

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Mol	Chain	Res	Type
1	A	87	GLN
1	A	174	ASN
1	A	226	GLN
1	A	253	GLN
2	B	51	HIS
2	B	83	ASN
1	D	86	ASN
1	D	141	GLN
1	D	174	ASN
1	D	226	GLN
1	D	253	GLN
2	E	83	ASN

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](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	GOL	B	105	-	5,5,5	0.98	0	5,5,5	0.79	0
6	SO4	D	304	-	4,4,4	0.48	0	6,6,6	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	E	102	-	4,4,4	0.51	0	6,6,6	0.42	0
7	GOL	A	309	-	5,5,5	0.70	0	5,5,5	0.31	0
6	SO4	D	306	-	4,4,4	0.42	0	6,6,6	0.28	0
5	EDO	A	303	-	3,3,3	0.62	0	2,2,2	0.26	0
5	EDO	B	101	-	3,3,3	0.53	0	2,2,2	0.32	0
6	SO4	A	307	-	4,4,4	0.54	0	6,6,6	0.14	0
6	SO4	D	305	-	4,4,4	0.54	0	6,6,6	0.40	0
6	SO4	A	306	-	4,4,4	0.63	0	6,6,6	0.24	0
5	EDO	D	303	-	3,3,3	0.44	0	2,2,2	0.65	0
5	EDO	A	302	-	3,3,3	0.43	0	2,2,2	0.07	0
5	EDO	B	103	-	3,3,3	0.46	0	2,2,2	0.17	0
7	GOL	A	310	-	5,5,5	0.59	0	5,5,5	0.31	0
7	GOL	D	308	-	5,5,5	0.68	0	5,5,5	0.83	0
6	SO4	A	305	-	4,4,4	0.53	0	6,6,6	0.50	0
6	SO4	E	101	-	4,4,4	0.53	0	6,6,6	0.44	0
7	GOL	D	307	-	5,5,5	0.61	0	5,5,5	0.62	0
5	EDO	B	102	-	3,3,3	0.57	0	2,2,2	0.28	0
7	GOL	A	308	-	5,5,5	0.43	0	5,5,5	0.34	0
6	SO4	A	304	-	4,4,4	0.38	0	6,6,6	0.43	0
7	GOL	B	106	-	5,5,5	0.32	0	5,5,5	0.47	0
5	EDO	D	302	-	3,3,3	0.70	0	2,2,2	1.04	0
6	SO4	B	104	-	4,4,4	0.41	0	6,6,6	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	302	-	-	0/1/1/1	-
5	EDO	B	101	-	-	1/1/1/1	-
5	EDO	B	103	-	-	0/1/1/1	-
7	GOL	B	105	-	-	4/4/4/4	-
7	GOL	B	106	-	-	1/4/4/4	-
7	GOL	A	310	-	-	2/4/4/4	-
7	GOL	D	308	-	-	2/4/4/4	-
7	GOL	A	309	-	-	3/4/4/4	-
5	EDO	D	302	-	-	1/1/1/1	-
7	GOL	D	307	-	-	3/4/4/4	-
5	EDO	D	303	-	-	0/1/1/1	-
5	EDO	B	102	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	303	-	-	1/1/1/1	-
7	GOL	A	308	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	309	GOL	O1-C1-C2-C3
7	B	105	GOL	O1-C1-C2-C3
7	B	105	GOL	C1-C2-C3-O3
7	A	310	GOL	O1-C1-C2-C3
7	D	307	GOL	O1-C1-C2-C3
7	D	307	GOL	C1-C2-C3-O3
7	D	308	GOL	O1-C1-C2-C3
7	A	309	GOL	O1-C1-C2-O2
7	A	310	GOL	O1-C1-C2-O2
7	D	308	GOL	O1-C1-C2-O2
5	A	303	EDO	O1-C1-C2-O2
5	B	101	EDO	O1-C1-C2-O2
7	B	105	GOL	O1-C1-C2-O2
7	B	105	GOL	O2-C2-C3-O3
7	D	307	GOL	O1-C1-C2-O2
7	A	308	GOL	O1-C1-C2-C3
5	D	302	EDO	O1-C1-C2-O2
7	B	106	GOL	O1-C1-C2-C3
7	A	309	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	302	EDO	1	0
7	D	308	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.34	5 (1%) 67 64	21, 37, 57, 77	0
1	D	276/276 (100%)	0.32	5 (1%) 67 64	16, 34, 55, 76	1 (0%)
2	B	100/100 (100%)	0.24	1 (1%) 79 76	19, 31, 52, 72	0
2	E	100/100 (100%)	0.26	3 (3%) 52 49	19, 33, 56, 77	0
3	C	9/9 (100%)	0.19	0 100 100	25, 30, 33, 39	0
3	F	9/9 (100%)	0.15	0 100 100	23, 30, 37, 38	0
All	All	770/770 (100%)	0.30	14 (1%) 67 64	16, 34, 56, 77	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	225	THR	4.0
1	D	275	GLU	3.8
1	A	275	GLU	3.5
1	D	276	PRO	3.2
2	E	98	ASP	3.0
1	A	39	ASP	2.9
2	E	74	GLU	2.8
1	A	32	GLN	2.5
1	D	1	GLY	2.4
1	D	267	PRO	2.3
1	A	276	PRO	2.2
2	B	99	MET	2.2
1	A	230	LEU	2.0
2	E	97	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
6	SO4	A	307	5/5	0.31	0.23	85,89,93,94	0
6	SO4	D	306	5/5	0.59	0.18	80,84,96,100	0
7	GOL	A	308	6/6	0.70	0.15	50,51,54,54	0
7	GOL	A	309	6/6	0.70	0.25	48,50,54,56	0
7	GOL	B	105	6/6	0.70	0.25	35,40,40,41	0
7	GOL	A	310	6/6	0.74	0.18	45,49,53,56	0
7	GOL	D	307	6/6	0.74	0.19	44,49,50,54	0
7	GOL	B	106	6/6	0.76	0.13	45,50,51,53	0
6	SO4	A	305	5/5	0.76	0.17	49,50,52,55	0
5	EDO	D	302	4/4	0.81	0.21	35,38,39,43	0
6	SO4	D	305	5/5	0.81	0.31	51,58,60,67	0
6	SO4	A	306	5/5	0.81	0.14	47,48,52,60	0
5	EDO	B	102	4/4	0.85	0.14	45,47,48,49	0
6	SO4	E	102	5/5	0.85	0.26	49,53,58,60	0
7	GOL	D	308	6/6	0.85	0.28	44,47,50,50	0
5	EDO	B	101	4/4	0.86	0.15	37,38,40,40	0
5	EDO	B	103	4/4	0.86	0.14	44,50,51,51	0
5	EDO	A	303	4/4	0.87	0.13	36,40,41,43	0
6	SO4	E	101	5/5	0.88	0.32	61,62,63,65	0
5	EDO	D	303	4/4	0.88	0.24	32,35,36,39	0
6	SO4	B	104	5/5	0.88	0.26	57,58,69,70	0
4	NA	A	301	1/1	0.89	0.09	31,31,31,31	0
4	NA	D	301	1/1	0.90	0.20	28,28,28,28	0
6	SO4	D	304	5/5	0.91	0.11	39,40,46,49	0
5	EDO	A	302	4/4	0.95	0.14	23,26,27,30	0
6	SO4	A	304	5/5	0.97	0.13	32,33,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.