



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 10:52 PM EDT

PDB ID : 6SS8  
Title : Human Leukocyte Antigen Class I A02 Carrying LLWNGPIAV  
Authors : Rizkallah, P.J.; Bovay, A.  
Deposited on : 2019-09-06  
Resolution : 2.24 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

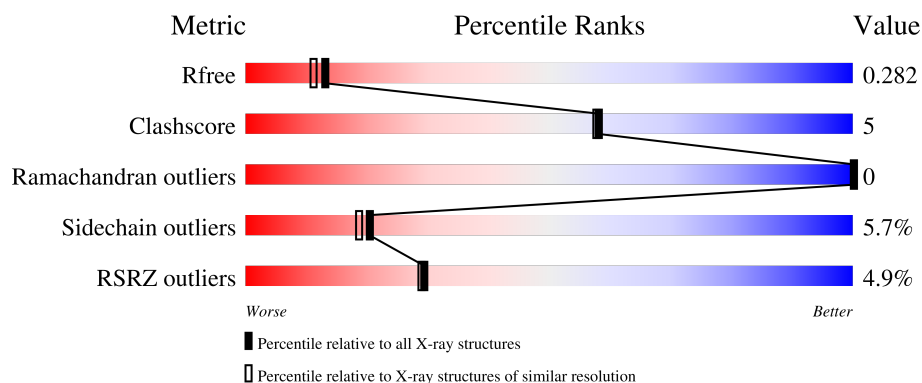
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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))
$R_{free}$	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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  $\geq 3$ , 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>5%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	D	276	<div> <div>6%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
2	B	100	<div> <div>3%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	E	100	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
3	C	9	<div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	9	 89%11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	D	302	-	-	-	X
7	PEG	B	106	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6718 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	0	0
			2254	1408	410	427	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			846	539	143	160	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-ASN-GLY-PRO-ILE-ALA-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			70	48	11	11			
3	F	9	Total	C	N	O	0	0	0
			70	48	11	11			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

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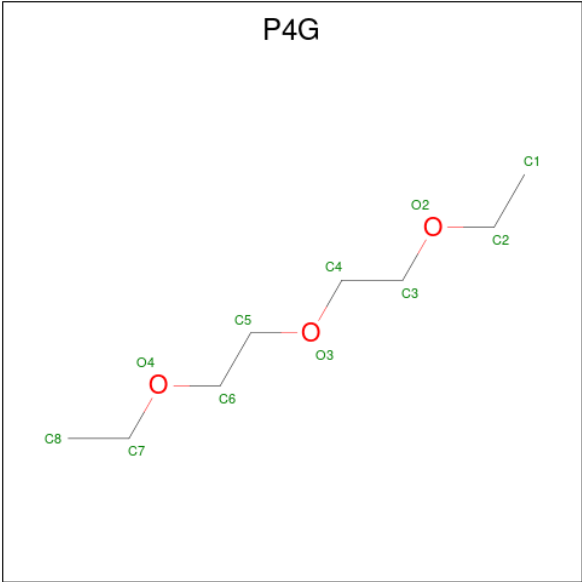
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula:  $C_8H_{18}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			11	8	3		

- Molecule 9 is water.

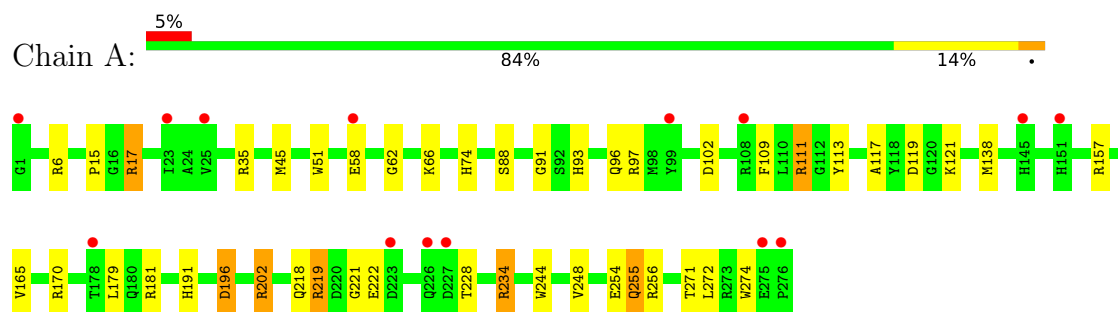
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	73	Total	O	0	0
			73	73		
9	B	49	Total	O	0	0
			49	49		
9	C	3	Total	O	0	0
			3	3		
9	D	88	Total	O	0	0
			88	88		
9	E	34	Total	O	0	0
			34	34		
9	F	2	Total	O	0	0
			2	2		



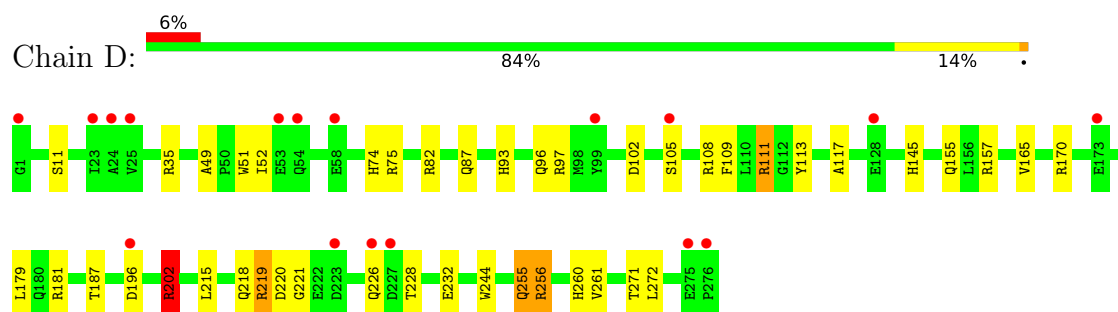
### 3 Residue-property plots [i](#)

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.

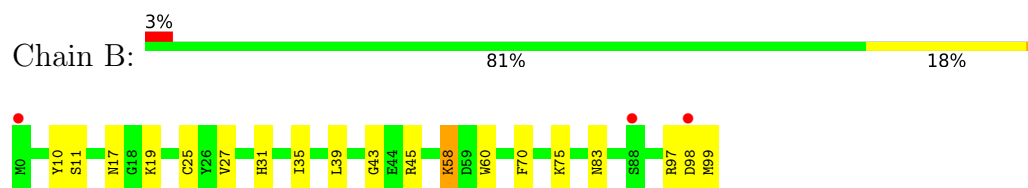
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



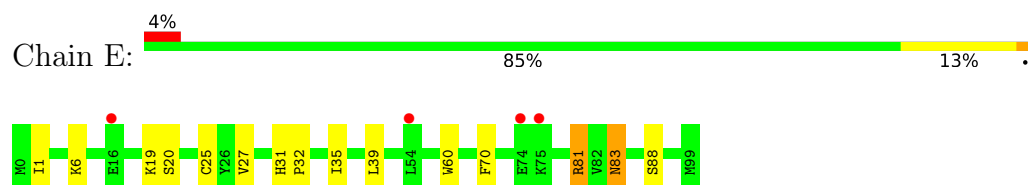
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




- Molecule 3: LEU-LEU-TRP-ASN-GLY-PRO-ILE-ALA-VAL

Chain C:  67% 33%



● Molecule 3: LEU-LEU-TRP-ASN-GLY-PRO-ILE-ALA-VAL

Chain F:  89% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.11Å 168.62Å 48.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.54 – 2.24 29.53 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.54-2.24) 98.3 (29.53-2.24)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.228 , 0.277 0.233 , 0.282	Depositor DCC
$R_{free}$ test set	2437 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6718	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.74 % 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 1.2425e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, SO4, P4G, GOL, PEG

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	0.73	0/2320	0.86	0/3149
1	D	0.76	0/2320	0.90	2/3149 (0.1%)
2	B	0.76	0/869	0.85	0/1173
2	E	0.76	0/860	0.89	0/1162
3	C	0.84	0/72	0.91	0/98
3	F	0.77	0/72	0.88	0/98
All	All	0.75	0/6513	0.88	2/8829 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	D	0	6
2	B	0	2
2	E	0	1
All	All	0	17

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	ARG	NE-CZ-NH1	-10.14	115.23	120.30
1	D	202	ARG	NE-CZ-NH2	8.66	124.63	120.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ARG	Sidechain
1	A	17	ARG	Sidechain
1	A	170	ARG	Sidechain
1	A	202	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	234	ARG	Sidechain
1	A	256	ARG	Sidechain
1	A	6	ARG	Sidechain
2	B	45	ARG	Sidechain
2	B	98	ASP	Peptide
1	D	108	ARG	Sidechain
1	D	170	ARG	Sidechain
1	D	202	ARG	Sidechain
1	D	219	ARG	Sidechain
1	D	256	ARG	Sidechain
1	D	75	ARG	Sidechain
2	E	81	ARG	Sidechain

## 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	21	0
1	D	2254	0	2103	21	0
2	B	846	0	815	13	0
2	E	837	0	803	12	0
3	C	70	0	75	2	0
3	F	70	0	75	0	0
4	A	6	0	8	1	0
4	B	12	0	16	1	0
4	D	24	0	32	1	0
4	E	12	0	16	0	0
5	A	4	0	6	0	0
6	A	15	0	0	0	0
6	B	15	0	0	1	0
6	D	5	0	0	0	0
6	E	20	0	0	0	0
7	B	7	0	10	0	0
7	D	7	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	11	0	18	2	0
9	A	73	0	0	1	0
9	B	49	0	0	2	0
9	C	3	0	0	0	0
9	D	88	0	0	1	0
9	E	34	0	0	2	0
9	F	2	0	0	0	0
All	All	6718	0	6090	60	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 5.

All (60) 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)
2:B:58[B]:LYS:H	2:B:58[B]:LYS:HE2	1.55	0.71
1:A:102:ASP:OD2	1:A:111:ARG:NH2	2.25	0.69
1:A:17:ARG:NH1	9:A:401:HOH:O	2.27	0.67
1:D:102:ASP:OD2	1:D:111:ARG:NH2	2.24	0.66
1:D:87:GLN:HE21	8:D:307:P4G:H72	1.61	0.65
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.81	0.64
1:D:220:ASP:OD2	1:D:256:ARG:NH1	2.32	0.63
2:B:58[B]:LYS:H	2:B:58[B]:LYS:CE	2.13	0.62
1:D:145:HIS:HB3	4:D:302:GOL:H2	1.82	0.61
1:A:88:SER:OG	4:A:301:GOL:H2	2.01	0.60
2:E:31:HIS:HD2	9:E:206:HOH:O	1.84	0.60
2:B:31:HIS:HD2	9:B:220:HOH:O	1.85	0.59
1:A:138:MET:HE2	2:E:81:ARG:HD3	1.85	0.57
2:B:17:ASN:OD1	2:B:97:ARG:NH2	2.29	0.57
1:D:96:GLN:OE1	2:E:31:HIS:HE1	1.88	0.56
2:B:31:HIS:CD2	9:B:220:HOH:O	2.58	0.55
1:A:255:GLN:OE1	1:A:274:TRP:O	2.24	0.55
2:B:43:GLY:HA2	4:B:102:GOL:H31	1.88	0.55
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.42	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.43	0.53
1:A:218:GLN:OE1	1:A:221:GLY:HA2	2.09	0.52
2:E:31:HIS:CD2	9:E:206:HOH:O	2.60	0.52
1:D:271:THR:O	1:D:272:LEU:HD23	2.09	0.52
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.45	0.52
1:D:218:GLN:OE1	1:D:221:GLY:HA2	2.09	0.52
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLN:HE21	8:D:307:P4G:C7	2.23	0.52
1:D:93:HIS:CD2	7:D:306:PEG:H11	2.45	0.51
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.46	0.51
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.96	0.49
2:B:27:VAL:HG11	2:B:35:ILE:CD1	2.43	0.49
2:E:27:VAL:HG11	2:E:35:ILE:CD1	2.43	0.48
2:B:11:SER:O	6:B:104:SO4:O4	2.32	0.48
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.32	0.48
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.95	0.48
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.49	0.47
1:D:187:THR:HB	1:D:272:LEU:HD11	1.96	0.47
1:D:82:ARG:HB2	7:D:306:PEG:H12	1.97	0.46
2:B:27:VAL:HG11	2:B:35:ILE:HD13	1.97	0.46
1:A:138:MET:HE2	2:E:81:ARG:CD	2.45	0.46
1:D:255:GLN:HB3	9:D:471:HOH:O	2.16	0.46
1:A:271:THR:O	1:A:272:LEU:HD23	2.15	0.45
1:A:109:PHE:HB2	1:A:165:VAL:HG21	1.98	0.45
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.35	0.45
3:C:5:GLY:N	3:C:6:PRO:CD	2.81	0.44
2:E:31:HIS:CD2	2:E:32:PRO:HA	2.53	0.43
2:E:83:ASN:HD22	2:E:83:ASN:HA	1.67	0.43
1:A:196:ASP:OD2	1:A:196:ASP:N	2.53	0.42
1:D:109:PHE:HB2	1:D:165:VAL:HG21	2.02	0.42
1:A:62:GLY:O	1:A:66:LYS:HG3	2.20	0.42
1:D:49:ALA:O	1:D:52:ILE:HG22	2.19	0.41
1:D:215:LEU:HD23	1:D:261:VAL:HG22	2.03	0.41
1:D:232:GLU:OE2	2:E:6:LYS:NZ	2.53	0.41
2:E:27:VAL:HG11	2:E:35:ILE:HD13	2.01	0.41
1:D:218:GLN:NE2	1:D:260:HIS:CD2	2.88	0.41
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.03	0.41
1:A:234:ARG:HD2	2:B:10:TYR:CE1	2.56	0.41
1:A:191:HIS:HE1	1:A:254:GLU:OE1	2.05	0.40
1:A:15:PRO:HG3	1:A:91:GLY:O	2.21	0.40
1:A:45:MET:CE	3:C:2:LEU:HD11	2.51	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	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
1	D	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
2	B	99/100 (99%)	97 (98%)	2 (2%)	0	100	100
2	E	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	759/770 (99%)	735 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/232 (100%)	220 (95%)	12 (5%)	23	22
1	D	232/232 (100%)	219 (94%)	13 (6%)	21	19
2	B	96/95 (101%)	89 (93%)	7 (7%)	14	10
2	E	95/95 (100%)	89 (94%)	6 (6%)	18	15
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	6 (86%)	1 (14%)	3	1
All	All	669/668 (100%)	630 (94%)	39 (6%)	20	18



All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	58	GLU
1	A	111	ARG
1	A	113	TYR
1	A	121	LYS
1	A	181	ARG
1	A	196	ASP
1	A	219	ARG
1	A	222	GLU
1	A	228	THR
1	A	248	VAL
1	A	255	GLN
2	B	19	LYS
2	B	58[A]	LYS
2	B	58[B]	LYS
2	B	70	PHE
2	B	75	LYS
2	B	83	ASN
2	B	99	MET
1	D	11	SER
1	D	35	ARG
1	D	105	SER
1	D	111	ARG
1	D	113	TYR
1	D	155	GLN
1	D	157	ARG
1	D	181	ARG
1	D	196	ASP
1	D	219	ARG
1	D	226	GLN
1	D	228	THR
1	D	255	GLN
2	E	1	ILE
2	E	19	LYS
2	E	20	SER
2	E	70	PHE
2	E	83	ASN
2	E	88	SER
3	F	7	ILE

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

Mol	Chain	Res	Type
1	A	74	HIS
1	A	86	ASN
1	A	93	HIS
1	A	174	ASN
1	A	191	HIS
1	A	192	HIS
1	A	226	GLN
1	A	253	GLN
1	A	255	GLN
2	B	31	HIS
2	B	83	ASN
1	D	74	HIS
1	D	86	ASN
1	D	87	GLN
1	D	174	ASN
1	D	226	GLN
1	D	253	GLN
2	E	31	HIS
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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 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	$\# Z  > 2$
4	GOL	D	302	-	5,5,5	0.62	0	5,5,5	0.49	0
4	GOL	D	304	-	5,5,5	0.38	0	5,5,5	0.55	0
6	SO4	E	104	-	4,4,4	0.35	0	6,6,6	0.25	0
7	PEG	D	306	-	6,6,6	0.91	0	5,5,5	1.10	0
8	P4G	D	307	-	10,10,10	0.60	0	9,9,9	0.58	0
6	SO4	E	106	-	4,4,4	0.40	0	6,6,6	0.21	0
5	EDO	A	302	-	3,3,3	0.58	0	2,2,2	0.16	0
6	SO4	B	105	-	4,4,4	0.33	0	6,6,6	0.19	0
4	GOL	E	101	-	5,5,5	0.48	0	5,5,5	1.20	1 (20%)
6	SO4	D	305	-	4,4,4	0.49	0	6,6,6	0.21	0
4	GOL	E	102	-	5,5,5	0.87	0	5,5,5	0.65	0
4	GOL	D	301	-	5,5,5	0.44	0	5,5,5	0.44	0
6	SO4	A	305	-	4,4,4	0.39	0	6,6,6	0.27	0
6	SO4	B	103	-	4,4,4	0.54	0	6,6,6	0.30	0
4	GOL	B	102	-	5,5,5	0.78	0	5,5,5	0.72	0
4	GOL	B	101	-	5,5,5	0.77	0	5,5,5	0.58	0
4	GOL	D	303	-	5,5,5	0.43	0	5,5,5	0.62	0
6	SO4	E	103	-	4,4,4	0.34	0	6,6,6	0.39	0
6	SO4	A	304	-	4,4,4	0.43	0	6,6,6	0.57	0
6	SO4	A	303	-	4,4,4	0.55	0	6,6,6	0.52	0
6	SO4	B	104	-	4,4,4	0.41	0	6,6,6	0.52	0
4	GOL	A	301	-	5,5,5	0.78	0	5,5,5	0.59	0
7	PEG	B	106	-	6,6,6	0.57	0	5,5,5	0.30	0
6	SO4	E	105	-	4,4,4	0.35	0	6,6,6	0.28	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
4	GOL	E	102	-	-	2/4/4/4	-
4	GOL	D	302	-	-	4/4/4/4	-
4	GOL	D	301	-	-	2/4/4/4	-
4	GOL	D	304	-	-	2/4/4/4	-
7	PEG	D	306	-	-	2/4/4/4	-
4	GOL	B	102	-	-	0/4/4/4	-
8	P4G	D	307	-	-	4/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	301	-	-	3/4/4/4	-
7	PEG	B	106	-	-	2/4/4/4	-
4	GOL	B	101	-	-	2/4/4/4	-
5	EDO	A	302	-	-	1/1/1/1	-
4	GOL	D	303	-	-	2/4/4/4	-
4	GOL	E	101	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	101	GOL	O1-C1-C2	-2.39	98.74	110.20

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GOL	C1-C2-C3-O3
4	B	101	GOL	O1-C1-C2-C3
4	D	302	GOL	O1-C1-C2-C3
4	D	302	GOL	C1-C2-C3-O3
4	D	303	GOL	C1-C2-C3-O3
4	D	304	GOL	C1-C2-C3-O3
4	E	101	GOL	C1-C2-C3-O3
4	E	102	GOL	O1-C1-C2-O2
4	E	102	GOL	O1-C1-C2-C3
4	D	301	GOL	O2-C2-C3-O3
4	D	302	GOL	O2-C2-C3-O3
4	D	304	GOL	O2-C2-C3-O3
8	D	307	P4G	O3-C5-C6-O4
7	B	106	PEG	O1-C1-C2-O2
7	D	306	PEG	O2-C3-C4-O4
4	D	301	GOL	C1-C2-C3-O3
4	B	101	GOL	O1-C1-C2-O2
4	D	303	GOL	O2-C2-C3-O3
4	E	101	GOL	O2-C2-C3-O3
4	D	302	GOL	O1-C1-C2-O2
7	B	106	PEG	O2-C3-C4-O4
8	D	307	P4G	C5-C6-O4-C7
7	D	306	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
8	D	307	P4G	C3-C4-O3-C5
5	A	302	EDO	O1-C1-C2-O2
4	A	301	GOL	O2-C2-C3-O3
4	A	301	GOL	O1-C1-C2-C3
8	D	307	P4G	O2-C3-C4-O3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	GOL	1	0
7	D	306	PEG	2	0
8	D	307	P4G	2	0
4	B	102	GOL	1	0
6	B	104	SO4	1	0
4	A	301	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	276/276 (100%)	0.40	14 (5%) 28 27	21, 39, 68, 87	0
1	D	276/276 (100%)	0.37	17 (6%) 20 20	21, 39, 66, 86	0
2	B	100/100 (100%)	0.22	3 (3%) 50 50	20, 33, 60, 75	0
2	E	100/100 (100%)	0.29	4 (4%) 38 38	19, 38, 61, 72	0
3	C	9/9 (100%)	0.69	0 100 100	30, 36, 39, 43	0
3	F	9/9 (100%)	0.82	0 100 100	29, 33, 47, 48	0
All	All	770/770 (100%)	0.36	38 (4%) 29 29	19, 38, 64, 87	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	GLN	4.9
1	A	227	ASP	4.8
1	A	223	ASP	4.6
1	A	275	GLU	4.4
1	D	275	GLU	3.7
1	A	178	THR	3.7
1	D	105	SER	3.4
1	D	227	ASP	3.4
1	A	276	PRO	3.4
2	B	0	MET	3.3
2	E	75	LYS	3.3
1	A	226	GLN	3.0
1	A	108	ARG	3.0
1	D	223	ASP	2.9
1	A	58	GLU	2.9
1	D	276	PRO	2.8
2	E	16	GLU	2.8
1	A	25	VAL	2.7
2	E	74	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	128	GLU	2.6
1	D	99	TYR	2.6
1	A	151	HIS	2.6
1	D	196	ASP	2.6
2	B	88	SER	2.6
1	A	145	HIS	2.5
1	D	54	GLN	2.4
2	B	98	ASP	2.4
1	D	23	ILE	2.3
1	D	25	VAL	2.3
1	D	58	GLU	2.2
1	D	1	GLY	2.2
1	D	24	ALA	2.1
1	D	53	GLU	2.1
1	D	173	GLU	2.1
2	E	54	LEU	2.1
1	A	99	TYR	2.1
1	A	1	GLY	2.1
1	A	23	ILE	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> 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
7	PEG	B	106	7/7	0.56	0.40	62,65,72,72	0
4	GOL	B	102	6/6	0.61	0.30	49,49,50,53	0
8	P4G	D	307	11/11	0.64	0.36	59,63,71,72	0
4	GOL	A	301	6/6	0.65	0.23	41,49,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	101	6/6	0.68	0.36	41,53,55,57	0
4	GOL	D	302	6/6	0.68	0.41	53,55,57,58	0
6	SO4	B	104	5/5	0.73	0.38	79,90,98,102	0
4	GOL	D	303	6/6	0.75	0.14	45,46,49,51	0
4	GOL	E	101	6/6	0.78	0.19	33,36,40,45	0
7	PEG	D	306	7/7	0.80	0.27	27,35,42,44	0
6	SO4	A	305	5/5	0.80	0.45	77,87,98,100	0
4	GOL	E	102	6/6	0.81	0.22	32,41,42,43	0
4	GOL	D	304	6/6	0.81	0.24	48,56,60,61	0
4	GOL	D	301	6/6	0.81	0.18	47,49,57,61	0
6	SO4	D	305	5/5	0.82	0.27	72,80,90,93	0
6	SO4	A	304	5/5	0.84	0.17	64,65,69,75	0
6	SO4	E	104	5/5	0.84	0.42	84,86,88,93	0
6	SO4	E	106	5/5	0.84	0.21	88,92,95,97	0
6	SO4	E	105	5/5	0.85	0.36	79,91,93,95	0
5	EDO	A	302	4/4	0.86	0.16	46,47,51,51	0
6	SO4	B	103	5/5	0.88	0.37	45,51,60,63	0
6	SO4	A	303	5/5	0.91	0.21	57,60,61,62	0
6	SO4	E	103	5/5	0.91	0.43	55,61,70,70	0
6	SO4	B	105	5/5	0.92	0.37	74,76,80,83	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.