



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:39 AM UTC

PDB ID : 4IHO / pdb_00004iho
Title : Crystal structure of H-2Db Y159F in complex with chimeric gp100
Authors : Uchtenhagen, H.; Stahl, E.; Achour, A.
Deposited on : 2012-12-19
Resolution : 2.80 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:

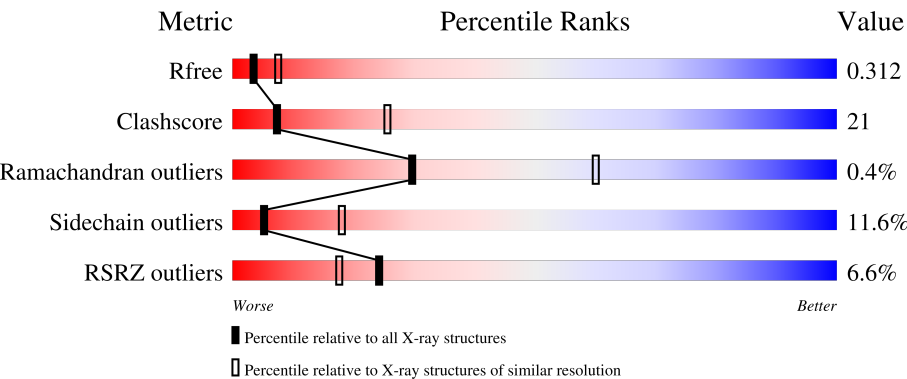
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	11% 60% 34% 5% .
1	D	276	6% 59% 33% 5% ..
2	B	99	% 62% 30% 6% .
2	E	99	2% 59% 32% 9%
3	C	9	56% 44%

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Mol	Chain	Length	Quality of chain
3	F	9	 44% 44% 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	B	101	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6397 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	71	1	0
			2247	1418	399	421	9			
1	D	272	Total	C	N	O	S	29	0	0
			2232	1408	395	420	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	PHE	TYR	engineered mutation	UNP P01899
D	159	PHE	TYR	engineered mutation	UNP P01899

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	1	0
			810	517	135	151	7			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	SEE REMARK 999	UNP P01887
E	85	ASP	ALA	SEE REMARK 999	UNP P01887

- Molecule 3 is a protein called NONAMERIC PEPTIDE CHIMERIC GP100.

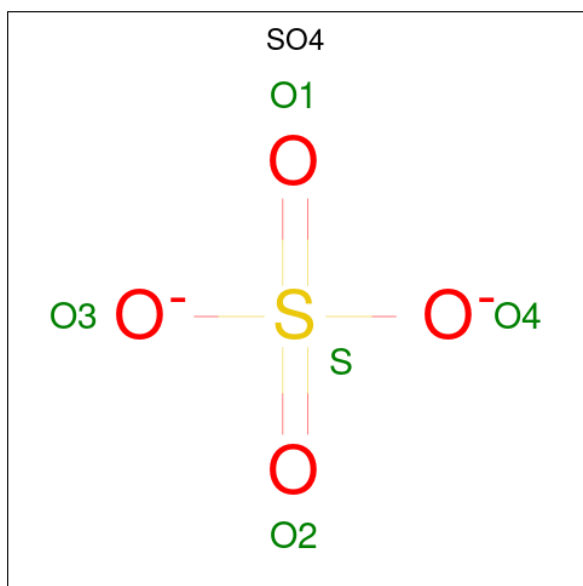
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			79	48	15	16			
3	F	9	Total	C	N	O	0	0	0
			79	48	15	16			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

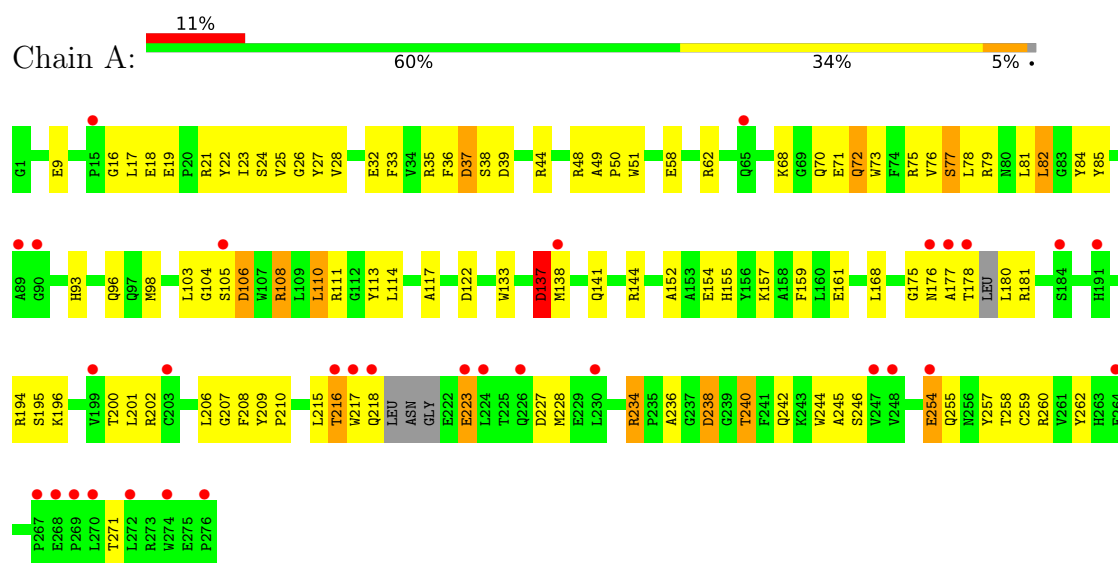
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	25	Total	O		0	0
			25	25			
6	B	25	Total	O		0	0
			25	25			
6	C	2	Total	O		0	0
			2	2			
6	D	24	Total	O		0	0
			24	24			
6	E	30	Total	O		0	0
			30	30			

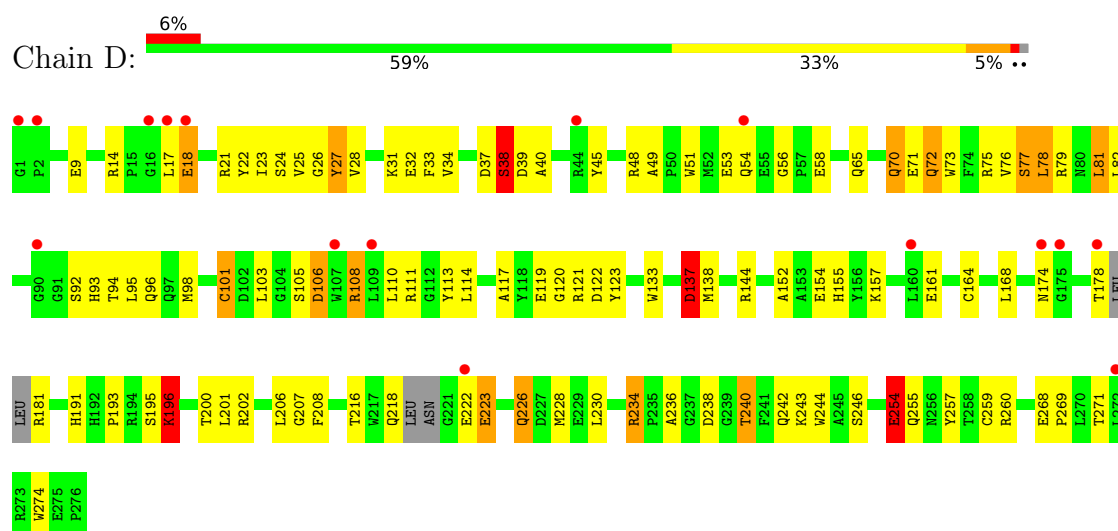
3 Residue-property plots [i](#)

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: H-2 class I histocompatibility antigen, D-B alpha chain

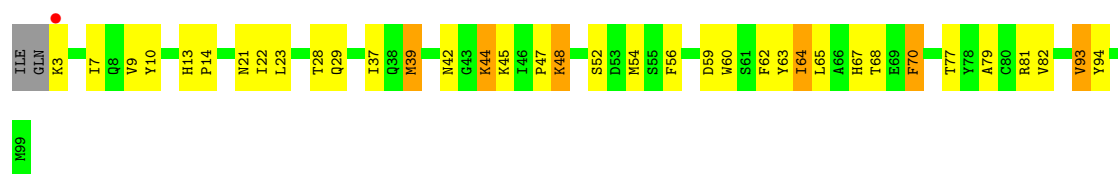


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

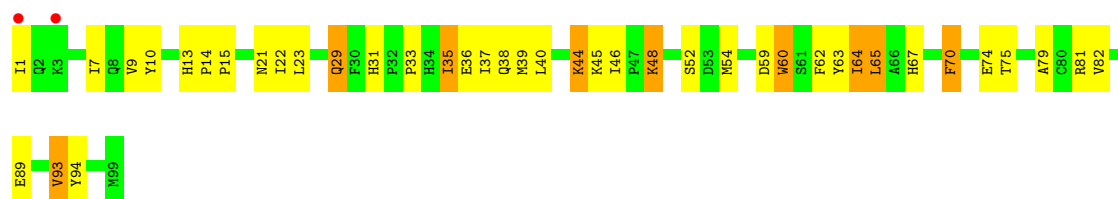


- Molecule 2: Beta-2-microglobulin





- Molecule 2: Beta-2-microglobulin



- Molecule 3: NONAMERIC PEPTIDE CHIMERIC GP100



- Molecule 3: NONAMERIC PEPTIDE CHIMERIC GP100



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.66Å 146.01Å 187.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.10 – 2.80 42.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (42.10-2.80) 97.3 (42.10-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.249 , 0.305 0.251 , 0.312	Depositor DCC
R_{free} test set	1537 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6397	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	0.70	0/2312	1.04	11/3134 (0.4%)
1	D	0.64	1/2297 (0.0%)	0.99	14/3114 (0.4%)
2	B	0.76	0/839	0.99	0/1138
2	E	0.78	0/847	1.06	3/1148 (0.3%)
3	C	0.93	0/81	0.94	0/108
3	F	1.38	0/81	0.95	0/108
All	All	0.72	1/6457 (0.0%)	1.02	28/8750 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	81	LEU	CA-C	-5.84	1.45	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	GLU	CB-CG-CD	8.94	127.80	112.60
1	A	216	THR	N-CA-C	7.33	120.36	108.34
1	A	196	LYS	N-CA-C	7.25	121.67	111.52
1	D	226	GLN	N-CA-C	7.18	119.19	111.36
1	A	216	THR	CB-CA-C	-6.86	99.17	110.14
1	A	255	GLN	N-CA-C	6.74	119.46	111.71
1	A	176	ASN	N-CA-C	6.70	118.46	111.03
2	E	46	ILE	CA-C-N	6.38	127.82	119.84
2	E	46	ILE	C-N-CA	6.38	127.82	119.84
1	D	255	GLN	N-CA-C	6.24	119.73	111.75
1	D	18	GLU	CB-CA-C	-6.16	109.48	116.63
1	D	38	SER	N-CA-C	6.15	119.88	112.38
1	D	223	GLU	N-CA-C	5.93	119.75	111.74
1	A	177	ALA	N-CA-C	-5.88	106.14	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	GLY	N-CA-C	-5.75	106.58	116.01
2	E	29	GLN	N-CA-C	5.66	119.38	111.74
1	A	208	PHE	N-CA-C	5.53	118.02	110.55
1	D	254	GLU	N-CA-C	5.50	117.35	111.36
1	A	227	ASP	CA-CB-CG	5.48	118.08	112.60
1	D	56	GLY	CA-C-N	5.40	125.73	119.47
1	D	56	GLY	C-N-CA	5.40	125.73	119.47
1	D	65	GLN	N-CA-C	-5.39	105.30	111.07
1	D	70	GLN	N-CA-C	-5.18	105.25	112.45
1	D	196	LYS	N-CA-C	5.11	118.67	111.52
1	D	82	LEU	N-CA-C	-5.08	105.74	111.28
1	D	119	GLU	N-CA-C	-5.05	106.70	112.86
1	A	37	ASP	N-CA-C	5.02	116.77	108.13
1	D	208	PHE	N-CA-C	5.01	117.15	110.53

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	2247	0	2115	91	0
1	D	2232	0	2097	88	0
2	B	810	0	780	38	0
2	E	821	0	796	38	0
3	C	79	0	70	5	0
3	F	79	0	70	9	0
4	A	12	0	16	4	0
4	B	6	0	8	5	0
5	A	5	0	0	0	0
6	A	25	0	0	6	0
6	B	25	0	0	1	0
6	C	2	0	0	0	0
6	D	24	0	0	5	0
6	E	30	0	0	3	0
All	All	6397	0	5952	246	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 21.

All (246) 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:47:PRO:HG2	2:B:48:LYS:HD2	1.29	1.11
1:A:216:THR:OG1	1:A:260:ARG:HB2	1.50	1.10
2:E:36:GLU:HB3	6:E:107:HOH:O	1.52	1.05
1:D:25:VAL:HG12	1:D:27:TYR:HE1	1.24	1.02
2:B:39:MET:HE2	2:B:68:THR:HG22	1.42	1.01
2:E:48:LYS:H	2:E:48:LYS:HD2	1.28	0.96
1:A:195:SER:HB2	6:A:409:HOH:O	1.64	0.96
1:D:25:VAL:CG1	1:D:27:TYR:HE1	1.77	0.95
1:D:137:ASP:HA	6:D:314:HOH:O	1.65	0.95
1:D:268:GLU:HG2	1:D:269:PRO:HD2	1.49	0.94
1:D:17:LEU:HD23	1:D:18:GLU:H	1.30	0.94
6:D:303:HOH:O	3:F:6:GLN:HB3	1.71	0.90
1:D:25:VAL:HG12	1:D:27:TYR:CE1	2.08	0.87
1:A:17:LEU:HD23	1:A:18:GLU:OE2	1.74	0.86
2:B:47:PRO:HG2	2:B:48:LYS:CD	2.06	0.85
1:A:216:THR:OG1	1:A:260:ARG:CB	2.24	0.85
2:E:48:LYS:HD2	2:E:48:LYS:N	1.86	0.85
1:D:17:LEU:CD2	1:D:18:GLU:H	1.89	0.84
1:D:101:CYS:HG	1:D:164:CYS:CB	1.91	0.83
1:A:27:TYR:HE2	6:A:401:HOH:O	1.63	0.82
1:D:26:GLY:C	1:D:27:TYR:HD1	1.89	0.80
2:B:3:LYS:HA	6:B:212:HOH:O	1.80	0.80
1:A:25:VAL:HG12	1:A:27:TYR:CE1	2.16	0.80
3:F:7:ASP:OD1	3:F:8:TRP:N	2.14	0.79
1:D:196:LYS:HD2	1:D:196:LYS:N	1.96	0.79
2:B:7:ILE:HG12	2:B:82:VAL:HG21	1.65	0.78
1:A:62:ARG:NH1	3:C:1:GLU:OE2	2.18	0.76
2:E:59:ASP:O	2:E:60:TRP:HB2	1.83	0.75
1:D:101:CYS:CB	1:D:164:CYS:SG	2.72	0.75
1:D:191:HIS:CE1	1:D:193:PRO:HG3	2.22	0.75
1:A:25:VAL:CG1	1:A:27:TYR:HE1	2.00	0.74
1:D:17:LEU:HD23	1:D:18:GLU:N	2.02	0.74
1:A:216:THR:HG1	1:A:260:ARG:HB2	1.52	0.73
1:A:25:VAL:CG1	1:A:27:TYR:CE1	2.71	0.73
1:D:191:HIS:HE1	1:D:193:PRO:HG3	1.53	0.72
1:D:17:LEU:CG	1:D:18:GLU:H	2.00	0.72
1:D:72:GLN:OE1	1:D:72:GLN:HA	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:MET:HE2	2:E:60:TRP:CH2	2.24	0.71
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.26	0.70
1:A:82:LEU:HD11	1:A:93:HIS:CD2	2.26	0.70
1:A:216:THR:HG1	1:A:260:ARG:CB	2.04	0.70
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.25	0.70
1:D:21:ARG:HG3	1:D:39:ASP:OD1	1.92	0.69
1:A:37:ASP:OD1	1:A:37:ASP:C	2.35	0.69
1:D:33:PHE:C	1:D:48:ARG:HB2	2.17	0.69
1:D:70:GLN:NE2	3:F:3:PRO:O	2.26	0.69
1:A:216:THR:O	1:A:260:ARG:N	2.22	0.68
1:D:207:GLY:O	1:D:240:THR:HB	1.92	0.68
1:D:37:ASP:C	1:D:37:ASP:OD1	2.37	0.68
1:A:98:MET:HE2	2:B:60:TRP:CZ2	2.29	0.67
2:B:47:PRO:CG	2:B:48:LYS:HD2	2.18	0.67
1:A:85:TYR:OH	1:A:137:ASP:OD2	2.14	0.65
4:A:302:GOL:H2	4:B:101:GOL:H11	1.78	0.65
1:D:268:GLU:HG2	1:D:269:PRO:CD	2.27	0.65
1:D:259:CYS:O	1:D:271:THR:HA	1.96	0.65
1:A:9:GLU:HG2	1:A:22:TYR:OH	1.97	0.64
1:D:33:PHE:CD2	1:D:34:VAL:HG13	2.32	0.64
1:D:32:GLU:OE2	1:D:48:ARG:HD2	1.97	0.64
1:D:25:VAL:CG1	1:D:27:TYR:CE1	2.69	0.64
1:A:259:CYS:O	1:A:271:THR:HA	2.00	0.62
1:D:234:ARG:NH1	1:D:242:GLN:OE1	2.33	0.62
1:A:27:TYR:CE2	6:A:401:HOH:O	2.45	0.62
2:B:52:SER:HB3	2:B:65:LEU:H	1.65	0.62
1:D:28:VAL:HG23	1:D:33:PHE:CE1	2.34	0.62
1:D:9:GLU:HG2	1:D:22:TYR:OH	1.99	0.61
2:B:21:ASN:HB3	2:B:70:PHE:HE1	1.64	0.61
1:A:108:ARG:HH11	1:A:108:ARG:HA	1.64	0.61
2:B:59:ASP:O	2:B:60:TRP:HB2	2.00	0.61
1:D:108:ARG:HA	1:D:108:ARG:HH11	1.65	0.61
1:A:98:MET:HE2	2:B:60:TRP:CH2	2.36	0.60
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.36	0.60
1:A:216:THR:OG1	1:A:260:ARG:CG	2.50	0.60
1:D:73:TRP:CZ2	3:F:8:TRP:HA	2.37	0.59
1:A:75[B]:ARG:NH1	6:A:414:HOH:O	2.34	0.59
1:D:121:ARG:HA	6:D:306:HOH:O	2.01	0.59
1:A:17:LEU:CG	1:A:18:GLU:H	2.16	0.58
1:A:49:ALA:O	1:A:51:TRP:N	2.36	0.58
2:E:52:SER:HB3	2:E:65:LEU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:GLU:HB3	2:E:75:THR:HG23	1.86	0.58
2:E:21:ASN:HB3	2:E:70:PHE:CE1	2.38	0.57
1:D:191:HIS:ND1	1:D:193:PRO:HD3	2.20	0.57
1:A:73:TRP:O	1:A:77:SER:OG	2.22	0.57
1:D:137:ASP:OD1	1:D:138:MET:N	2.37	0.57
2:B:48:LYS:HD2	2:B:48:LYS:N	2.19	0.57
2:E:79:ALA:HB2	2:E:94:TYR:CD2	2.39	0.57
1:A:25:VAL:HG11	1:A:27:TYR:HE1	1.70	0.57
1:A:33:PHE:C	1:A:48:ARG:HB2	2.30	0.57
2:B:56:PHE:HB3	2:B:62:PHE:CD2	2.40	0.57
2:B:54:MET:N	4:B:101:GOL:H2	2.20	0.56
1:A:21:ARG:HG3	1:A:39:ASP:OD1	2.06	0.56
1:A:216:THR:CG2	1:A:262:TYR:HE2	2.18	0.56
1:A:234:ARG:NH1	1:A:242:GLN:OE1	2.36	0.56
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.41	0.56
1:A:216:THR:OG1	1:A:216:THR:O	2.19	0.56
2:B:48:LYS:CD	2:B:48:LYS:H	2.19	0.56
2:E:63:TYR:HD2	6:E:103:HOH:O	1.89	0.56
1:D:155:HIS:CD2	3:F:6:GLN:HB2	2.41	0.56
1:A:82:LEU:HD11	1:A:93:HIS:HD2	1.72	0.55
1:A:23:ILE:N	1:A:23:ILE:HD12	2.21	0.55
1:D:103:LEU:HG	1:D:168:LEU:HD23	1.88	0.55
1:A:17:LEU:HG	1:A:18:GLU:H	1.72	0.55
2:E:21:ASN:HB2	6:E:106:HOH:O	2.07	0.55
2:E:37:ILE:HD13	2:E:64:ILE:HG21	1.87	0.55
1:D:120:GLY:HA3	2:E:31:HIS:CD2	2.42	0.55
2:B:54:MET:H	4:B:101:GOL:H2	1.72	0.54
2:B:79:ALA:HB2	2:B:94:TYR:CD2	2.43	0.53
1:A:25:VAL:HG11	1:A:27:TYR:CE1	2.43	0.53
1:A:35:ARG:NH2	2:B:54:MET:O	2.36	0.53
1:D:14:ARG:NH2	6:D:310:HOH:O	2.40	0.53
2:B:28:THR:O	2:B:29:GLN:HB2	2.08	0.53
2:B:48:LYS:CD	2:B:48:LYS:N	2.72	0.53
1:A:96:GLN:HB3	2:B:60:TRP:CZ3	2.44	0.53
1:A:216:THR:O	1:A:260:ARG:HG3	2.08	0.53
1:A:216:THR:HG21	1:A:262:TYR:HE2	1.75	0.52
1:D:17:LEU:CG	1:D:18:GLU:N	2.73	0.52
2:E:23:LEU:HD23	2:E:39:MET:HE2	1.91	0.52
1:A:194:ARG:HD2	1:A:195:SER:H	1.75	0.52
1:A:175:GLY:HA2	1:A:178:THR:HG23	1.92	0.51
1:D:196:LYS:HD2	1:D:196:LYS:H	1.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:ILE:HG13	2:E:36:GLU:H	1.74	0.51
1:A:27:TYR:CD1	1:A:32:GLU:HA	2.46	0.51
1:A:103:LEU:HG	1:A:168:LEU:HD23	1.93	0.51
2:B:39:MET:CE	2:B:68:THR:HG22	2.29	0.51
1:D:106:ASP:OD1	1:D:106:ASP:N	2.36	0.51
2:B:47:PRO:HG2	2:B:48:LYS:CE	2.41	0.51
1:A:133:TRP:HB2	1:A:144:ARG:HG3	1.92	0.50
1:A:159:PHE:CE2	3:C:3:PRO:HB3	2.46	0.50
1:A:44:ARG:NH1	6:A:420:HOH:O	2.41	0.50
1:D:133:TRP:HB2	1:D:144:ARG:HG3	1.92	0.50
1:A:106:ASP:CG	1:A:108:ARG:HG2	2.37	0.50
1:A:82:LEU:CD1	1:A:93:HIS:CD2	2.94	0.50
2:B:48:LYS:O	2:B:48:LYS:HG2	2.11	0.50
2:E:23:LEU:O	2:E:67:HIS:HA	2.12	0.49
1:A:207:GLY:O	1:A:240:THR:HB	2.12	0.49
1:A:111:ARG:HD3	1:A:113:TYR:CZ	2.47	0.49
1:D:238:ASP:OD1	1:D:238:ASP:N	2.39	0.49
2:E:7:ILE:HG12	2:E:82:VAL:HG21	1.93	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.49
1:A:72:GLN:OE1	1:A:72:GLN:HA	2.12	0.48
1:A:195:SER:CB	6:A:409:HOH:O	2.39	0.48
1:D:94:THR:HG21	2:E:31:HIS:CE1	2.48	0.48
1:D:98:MET:HE2	2:E:60:TRP:CZ2	2.48	0.48
2:B:23:LEU:O	2:B:67:HIS:HA	2.13	0.48
1:A:236:ALA:HB3	1:A:238:ASP:OD1	2.14	0.48
1:D:25:VAL:CG1	1:D:32:GLU:HG3	2.44	0.48
1:A:217:TRP:HA	1:A:258:THR:O	2.13	0.48
1:D:191:HIS:HB2	1:D:274:TRP:CE2	2.49	0.47
1:A:36:PHE:CD1	1:A:36:PHE:C	2.92	0.47
1:A:194:ARG:NH2	1:A:195:SER:HB3	2.29	0.47
4:A:302:GOL:C2	4:B:101:GOL:H11	2.44	0.47
2:E:21:ASN:O	2:E:70:PHE:HD1	1.97	0.47
2:B:56:PHE:HB3	2:B:62:PHE:CE2	2.49	0.47
2:E:9:VAL:HG23	2:E:93:VAL:HG22	1.96	0.47
1:A:234:ARG:HD3	2:B:10:TYR:CE1	2.49	0.47
1:D:26:GLY:C	1:D:27:TYR:CD1	2.80	0.47
1:D:40:ALA:HB1	6:D:311:HOH:O	2.14	0.47
1:D:234:ARG:HD3	2:E:10:TYR:CZ	2.49	0.47
1:D:236:ALA:HB3	1:D:238:ASP:OD1	2.14	0.47
2:B:44:LYS:HD3	2:B:44:LYS:HA	1.56	0.47
1:A:70:GLN:O	1:A:71:GLU:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ASP:OD1	2:E:60:TRP:NE1	2.46	0.47
2:B:42:ASN:HA	2:B:77:THR:HG1	1.81	0.46
2:E:31:HIS:CE1	2:E:62:PHE:HE1	2.33	0.46
1:D:23:ILE:N	1:D:23:ILE:HD12	2.30	0.46
1:D:178:THR:O	1:D:181:ARG:N	2.48	0.46
1:D:195:SER:OG	1:D:196:LYS:HD2	2.15	0.46
3:C:6:GLN:HE21	3:C:7:ASP:HB2	1.80	0.46
1:A:21:ARG:NE	1:A:23:ILE:HD11	2.30	0.46
1:D:81:LEU:HD23	1:D:81:LEU:HA	1.59	0.46
1:D:37:ASP:OD1	1:D:38:SER:N	2.49	0.46
1:D:58:GLU:CD	1:D:58:GLU:H	2.23	0.46
1:D:27:TYR:CD1	1:D:27:TYR:N	2.84	0.46
2:E:33:PRO:HB2	2:E:54:MET:HE2	1.98	0.46
1:A:155:HIS:CD2	3:C:6:GLN:HB2	2.51	0.46
1:A:238:ASP:OD1	1:A:238:ASP:N	2.46	0.46
1:D:33:PHE:O	1:D:48:ARG:HB2	2.16	0.45
1:D:70:GLN:O	1:D:71:GLU:C	2.57	0.45
2:B:48:LYS:HD2	2:B:48:LYS:H	1.78	0.45
2:E:33:PRO:HD3	2:E:62:PHE:CE1	2.51	0.45
1:A:17:LEU:HG	1:A:18:GLU:N	2.30	0.45
1:A:137:ASP:OD1	1:A:138:MET:N	2.50	0.45
4:A:302:GOL:H2	4:B:101:GOL:C1	2.47	0.45
1:D:72:GLN:HE22	1:D:75:ARG:NH1	2.14	0.45
1:D:123:TYR:CD1	1:D:123:TYR:C	2.95	0.45
1:A:157:LYS:NZ	1:A:161:GLU:OE2	2.49	0.45
1:D:218:GLN:CB	1:D:260:ARG:NH2	2.80	0.45
2:B:37:ILE:HD13	2:B:64:ILE:HG21	1.98	0.44
1:D:216:THR:OG1	1:D:260:ARG:HB2	2.17	0.44
1:A:28:VAL:HG23	1:A:33:PHE:CD1	2.52	0.44
2:E:33:PRO:HB3	2:E:62:PHE:CE2	2.53	0.44
3:F:6:GLN:CG	3:F:7:ASP:H	2.30	0.44
1:A:152:ALA:HA	3:C:6:GLN:OE1	2.17	0.44
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.52	0.44
1:D:73:TRP:CE2	3:F:8:TRP:HA	2.53	0.44
1:D:78:LEU:HD13	1:D:95:LEU:HB2	2.00	0.44
1:D:111:ARG:HD3	1:D:113:TYR:CZ	2.53	0.44
1:D:137:ASP:OD1	1:D:137:ASP:C	2.60	0.44
1:D:152:ALA:HA	3:F:6:GLN:NE2	2.32	0.44
2:E:21:ASN:HB3	2:E:70:PHE:HE1	1.81	0.44
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.53	0.43
2:E:48:LYS:O	2:E:48:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.19	0.43
2:E:13:HIS:O	2:E:14:PRO:C	2.61	0.43
1:A:122:ASP:OD1	2:B:60:TRP:NE1	2.38	0.43
1:A:106:ASP:OD1	1:A:106:ASP:N	2.35	0.43
1:A:215:LEU:HD23	1:A:245:ALA:HB3	2.00	0.43
1:D:230:LEU:HD13	1:D:243:LYS:HE3	2.01	0.43
1:D:157:LYS:NZ	1:D:161:GLU:OE2	2.50	0.43
2:E:45:LYS:HB3	2:E:45:LYS:HE2	1.81	0.43
1:A:76:VAL:O	1:A:79:ARG:N	2.48	0.43
2:B:28:THR:HG22	2:B:63:TYR:HB2	2.00	0.43
1:D:54:GLN:OE1	1:D:174:ASN:OD1	2.36	0.43
1:D:218:GLN:HB2	1:D:260:ARG:HH21	1.84	0.42
1:A:26:GLY:C	1:A:27:TYR:CD1	2.96	0.42
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.54	0.42
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.55	0.42
2:B:9:VAL:HG23	2:B:93:VAL:HG22	2.01	0.42
1:D:76:VAL:O	1:D:79:ARG:N	2.52	0.42
2:E:14:PRO:HA	2:E:15:PRO:HD3	1.95	0.42
1:D:201:LEU:O	1:D:246:SER:HA	2.20	0.42
2:E:44:LYS:HD3	2:E:44:LYS:HA	1.57	0.42
1:D:28:VAL:HG23	1:D:33:PHE:CD1	2.54	0.42
2:E:60:TRP:CE3	2:E:60:TRP:HA	2.55	0.42
1:D:96:GLN:HB3	2:E:60:TRP:CZ3	2.54	0.42
1:D:254:GLU:O	1:D:257:TYR:HD2	2.03	0.42
1:A:201:LEU:O	1:A:246:SER:HA	2.20	0.42
1:D:92:SER:O	1:D:93:HIS:ND1	2.53	0.42
3:F:7:ASP:OD1	3:F:7:ASP:C	2.64	0.41
1:D:73:TRP:O	1:D:77:SER:OG	2.34	0.41
1:A:26:GLY:O	1:A:27:TYR:HD1	2.03	0.41
1:A:85:TYR:CZ	4:A:301:GOL:H31	2.54	0.41
1:A:254:GLU:O	1:A:257:TYR:HD2	2.04	0.41
1:A:26:GLY:C	1:A:27:TYR:HD1	2.29	0.41
1:A:141:GLN:OE1	1:A:141:GLN:HA	2.20	0.41
1:A:133:TRP:O	1:A:144:ARG:HD2	2.21	0.41
2:B:13:HIS:O	2:B:14:PRO:C	2.63	0.41
1:A:49:ALA:O	1:A:50:PRO:C	2.64	0.40
1:D:49:ALA:O	1:D:51:TRP:N	2.54	0.40
1:D:133:TRP:O	1:D:144:ARG:HD2	2.21	0.40
1:A:37:ASP:OD1	1:A:38:SER:N	2.54	0.40
1:A:58:GLU:H	1:A:58:GLU:CD	2.27	0.40
2:E:35:ILE:HG13	2:E:36:GLU:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD23	1:A:84:TYR:HD2	1.86	0.40
1:A:104:GLY:CA	1:A:110:LEU:CD1	2.99	0.40
1:A:106:ASP:OD2	1:A:108:ARG:HG2	2.22	0.40
1:D:25:VAL:HG11	1:D:27:TYR:HE1	1.73	0.40

There are no symmetry-related clashes.

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	267/276 (97%)	255 (96%)	11 (4%)	1 (0%)	30	60
1	D	266/276 (96%)	257 (97%)	8 (3%)	1 (0%)	30	60
2	B	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
2	E	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	0	1 (14%)	0	0
All	All	740/768 (96%)	711 (96%)	26 (4%)	3 (0%)	30	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	6	GLN
1	D	137	ASP
1	A	137	ASP

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	232/234 (99%)	207 (89%)	25 (11%)	6	21
1	D	230/234 (98%)	203 (88%)	27 (12%)	5	18
2	B	93/94 (99%)	84 (90%)	9 (10%)	8	25
2	E	94/94 (100%)	79 (84%)	15 (16%)	2	9
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	7 (88%)	1 (12%)	4	15
All	All	665/672 (99%)	588 (88%)	77 (12%)	5	18

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	24	SER
1	A	68	LYS
1	A	72	GLN
1	A	77	SER
1	A	78	LEU
1	A	82	LEU
1	A	105	SER
1	A	106	ASP
1	A	108	ARG
1	A	110	LEU
1	A	114	LEU
1	A	137	ASP
1	A	154	GLU
1	A	180	LEU
1	A	181	ARG
1	A	200	THR
1	A	206	LEU
1	A	218	GLN
1	A	223	GLU
1	A	228	MET
1	A	234	ARG
1	A	238	ASP
1	A	240	THR
1	A	254	GLU
2	B	22	ILE

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Mol	Chain	Res	Type
2	B	39	MET
2	B	44	LYS
2	B	45	LYS
2	B	48	LYS
2	B	64	ILE
2	B	70	PHE
2	B	81	ARG
2	B	93	VAL
1	D	24	SER
1	D	27	TYR
1	D	31	LYS
1	D	38	SER
1	D	45	TYR
1	D	53	GLU
1	D	72	GLN
1	D	77	SER
1	D	78	LEU
1	D	101	CYS
1	D	105	SER
1	D	106	ASP
1	D	108	ARG
1	D	110	LEU
1	D	114	LEU
1	D	137	ASP
1	D	154	GLU
1	D	196	LYS
1	D	200	THR
1	D	206	LEU
1	D	222	GLU
1	D	223	GLU
1	D	226	GLN
1	D	228	MET
1	D	234	ARG
1	D	240	THR
1	D	254	GLU
2	E	1	ILE
2	E	22	ILE
2	E	29	GLN
2	E	35	ILE
2	E	38	GLN
2	E	40	LEU
2	E	44	LYS

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Mol	Chain	Res	Type
2	E	48	LYS
2	E	60	TRP
2	E	64	ILE
2	E	65	LEU
2	E	70	PHE
2	E	81	ARG
2	E	89	GLU
2	E	93	VAL
3	F	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	191	HIS
1	A	255	GLN
2	B	13	HIS
2	B	34	HIS
1	D	72	GLN
1	D	115	GLN
1	D	191	HIS
1	D	255	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](#)

4 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	A	301	-	5,5,5	0.50	0	5,5,5	0.53	0
4	GOL	B	101	-	5,5,5	0.88	0	5,5,5	1.26	1 (20%)
5	SO4	A	303	-	4,4,4	0.45	0	6,6,6	0.06	0
4	GOL	A	302	-	5,5,5	1.08	0	5,5,5	2.02	1 (20%)

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	A	301	-	-	4/4/4/4	-
4	GOL	B	101	-	-	2/4/4/4	-
4	GOL	A	302	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	GOL	C3-C2-C1	3.56	124.86	111.80
4	B	101	GOL	C3-C2-C1	2.74	121.85	111.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GOL	O1-C1-C2-C3
4	A	301	GOL	C1-C2-C3-O3
4	A	301	GOL	O2-C2-C3-O3
4	B	101	GOL	O2-C2-C3-O3
4	A	302	GOL	O1-C1-C2-O2
4	B	101	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	301	GOL	O1-C1-C2-O2
4	A	302	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GOL	1	0
4	B	101	GOL	5	0
4	A	302	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	272/276 (98%)	0.70	31 (11%) 10 7	14, 64, 135, 156	17 (6%)
1	D	272/276 (98%)	0.67	16 (5%) 28 21	21, 68, 115, 136	8 (2%)
2	B	97/99 (97%)	0.28	1 (1%) 79 72	29, 49, 80, 99	1 (1%)
2	E	99/99 (100%)	0.27	2 (2%) 65 56	20, 48, 78, 111	0
3	C	9/9 (100%)	0.06	0 100 100	28, 40, 55, 56	0
3	F	9/9 (100%)	0.24	0 100 100	12, 34, 61, 64	0
All	All	758/768 (98%)	0.57	50 (6%) 24 18	12, 59, 118, 156	26 (3%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	GLY	4.1
1	A	65	GLN	3.8
1	A	89	ALA	3.8
1	A	90	GLY	3.8
1	A	269	PRO	3.7
1	D	107	TRP	3.6
1	A	270	LEU	3.5
1	A	177	ALA	3.4
2	B	3	LYS	3.4
1	A	203	CYS	3.3
1	D	175	GLY	3.3
1	A	217	TRP	3.2
1	A	247	VAL	3.1
1	D	17	LEU	3.1
1	A	274	TRP	3.0
2	E	1	ILE	2.9
1	A	191	HIS	2.9
1	A	199	VAL	2.9
1	A	15	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	174	ASN	2.7
1	D	2	PRO	2.7
1	A	264	GLU	2.7
1	D	222	GLU	2.7
1	D	272	LEU	2.7
1	A	218	GLN	2.6
2	E	3	LYS	2.5
1	D	16	GLY	2.5
1	A	184	SER	2.5
1	A	176	ASN	2.5
1	A	267	PRO	2.5
1	D	109	LEU	2.4
1	A	276	PRO	2.4
1	D	44	ARG	2.4
1	A	216	THR	2.4
1	A	223	GLU	2.4
1	A	254	GLU	2.4
1	A	178	THR	2.4
1	D	178	THR	2.4
1	D	90	GLY	2.3
1	A	230	LEU	2.3
1	A	226	GLN	2.3
1	A	138	MET	2.2
1	D	54	GLN	2.2
1	A	224	LEU	2.2
1	A	105	SER	2.1
1	D	18	GLU	2.1
1	A	272	LEU	2.1
1	D	160	LEU	2.1
1	A	268	GLU	2.1
1	A	248	VAL	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	303	5/5	0.61	0.09	138,139,142,144	0
4	GOL	B	101	6/6	0.90	0.13	8,9,10,10	0
4	GOL	A	302	6/6	0.90	0.12	4,5,5,6	0
4	GOL	A	301	6/6	0.91	0.10	33,33,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.