



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 04:32 AM EDT

PDB ID : 4IHO  
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](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:

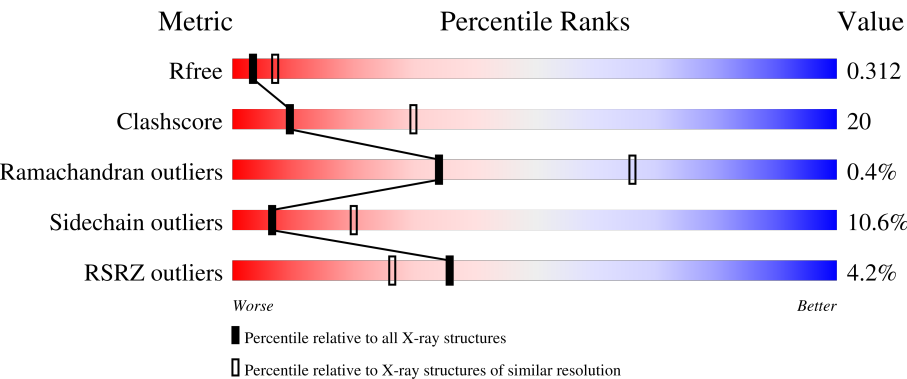
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

# 1 Overall quality at a glance 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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  $\geq 3$ , 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>8%</div><div><div></div><div>63%</div><div>31%</div><div>• •</div></div></div>
1	D	276	<div><div>3%</div><div><div></div><div>61%</div><div>33%</div><div>• •</div></div></div>
2	B	99	<div><div>%</div><div><div></div><div>67%</div><div>25%</div><div>6%</div><div>•</div></div></div>
2	E	99	<div><div>%</div><div><div></div><div>63%</div><div>30%</div><div>7%</div></div></div>
3	C	9	<div><div></div><div><div></div><div>56%</div><div>44%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	F	9	

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.

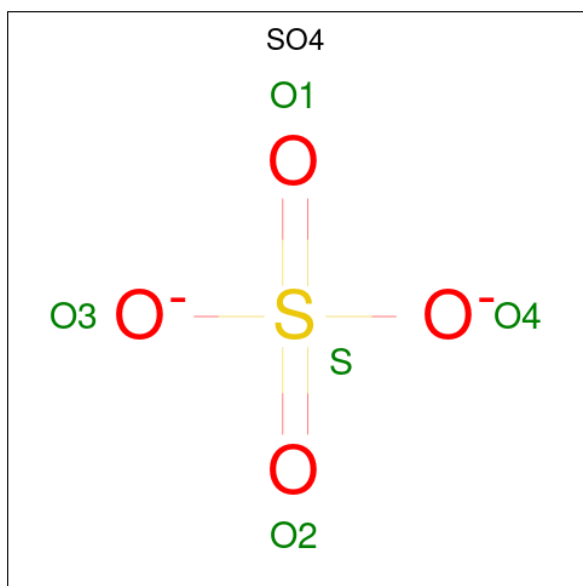
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			79	48	15	16			
3	F	9	Total	C	N	O	0	0	0
			79	48	15	16			

- Molecule 4 is GLYCEROL (three-letter code: 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 (three-letter code: SO4) (formula:  $O_4S$ ).



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

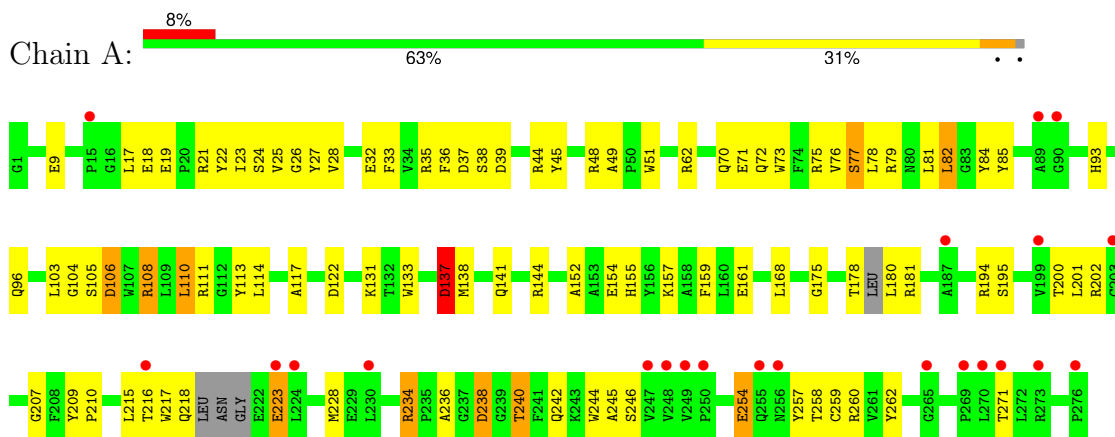
- Molecule 6 is water.

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			

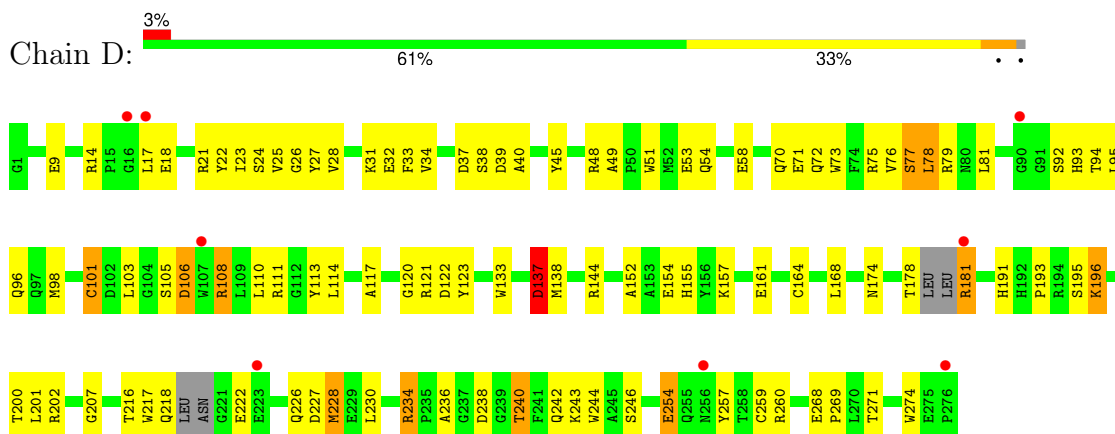
### 3 Residue-property plots [i](#)

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.

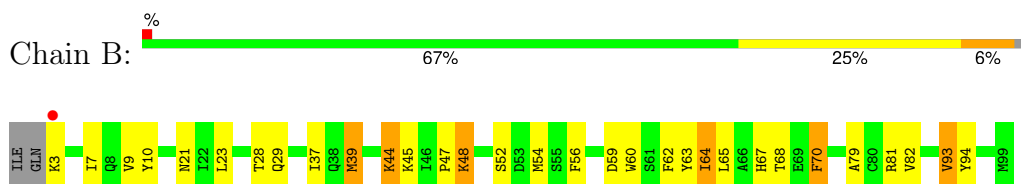
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



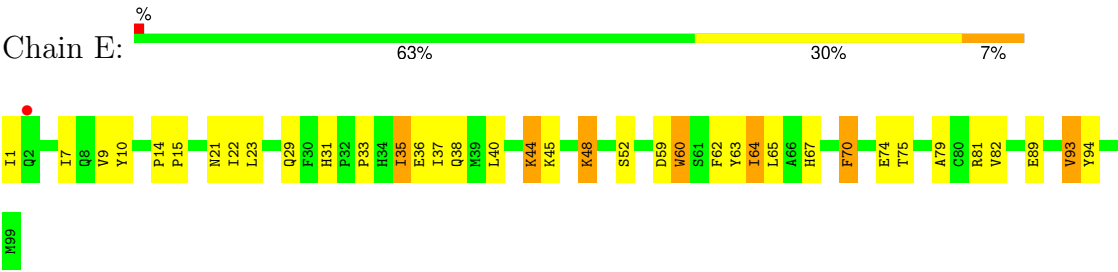
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



- 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, $\alpha$ , $\beta$ , $\gamma$	90.66Å 146.01Å 187.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.10 – 2.80 42.07 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (42.10-2.80) 97.4 (42.07-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.9	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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: 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	0.56	0/2312	0.72	1/3134 (0.0%)
1	D	0.50	0/2297	0.66	0/3114
2	B	0.54	0/839	0.73	1/1138 (0.1%)
2	E	0.57	0/847	0.72	0/1148
3	C	0.87	0/81	0.77	0/108
3	F	1.27	0/81	0.82	0/108
All	All	0.56	0/6457	0.70	2/8750 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	MET	CG-SD-CE	5.48	108.97	100.20
1	A	223	GLU	CB-CG-CD	5.04	127.80	114.20

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	85	0
1	D	2232	0	2097	88	0
2	B	810	0	780	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	821	0	796	34	0
3	C	79	0	70	5	0
3	F	79	0	70	8	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	235	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 20.

All (235) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:26:GLY:C	1:D:27:TYR:HD1	1.89	0.76
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
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: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
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:A:37:ASP:OD1	1:A:37:ASP:C	2.35	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:D:33:PHE:C	1:D:48:ARG:HB2	2.17	0.64
1:D:37:ASP:C	1:D:37:ASP:OD1	2.37	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:MET:CE	2:B:68:THR:HG22	2.29	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: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:B:39:MET:HE1	2:B:68:THR:HG22	1.85	0.58
2:E:52:SER:HB3	2:E:65:LEU:H	1.69	0.58
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:33:PHE:C	1:A:48:ARG:HB2	2.30	0.52
1:D:17:LEU:CG	1:D:18:GLU:N	2.73	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
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
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: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:N	1:D:238:ASP:OD1	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:122:ASP:OD1	2:E:60:TRP:NE1	2.46	0.47
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
1:D:217:TRP:H	1:D:228:MET:HE1	1.79	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
2:B:39:MET:HE2	2:B:68:THR:HG22	1.97	0.46
1:D:37:ASP:OD1	1:D:38:SER:N	2.49	0.46
1:D:27:TYR:N	1:D:27:TYR:CD1	2.84	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
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:A:157:LYS:NZ	1:A:161:GLU:OE2	2.49	0.45
1:A:106:ASP:CG	1:A:108:ARG:HG2	2.37	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:152:ALA:HA	3:F:6:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.19	0.43
1:A:122:ASP:OD1	2:B:60:TRP:NE1	2.38	0.43
1:D:98:MET:HE2	1:D:98:MET:HB2	1.77	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:26:GLY:C	1:D:27:TYR:CD1	2.80	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:A:36:PHE:CD1	1:A:36:PHE:C	2.92	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: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:A:70:GLN:O	1:A:71:GLU:C	2.57	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
1:D:98:MET:HE2	2:E:60:TRP:CH2	2.54	0.42
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:D:58:GLU:H	1:D:58:GLU:CD	2.23	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:141:GLN:OE1	1:A:141:GLN:HA	2.20	0.41
1:D:70:GLN:O	1:D:71:GLU:C	2.57	0.41
1:A:133:TRP:O	1:A:144:ARG:HD2	2.21	0.41
1:D:49:ALA:O	1:D:51:TRP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:123:TYR:CD1	1:D:123:TYR:C	2.95	0.40
2:E:35:ILE:HG13	2:E:36:GLU:N	2.37	0.40
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

### 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	267/276 (97%)	255 (96%)	11 (4%)	1 (0%)	34	66
1	D	266/276 (96%)	257 (97%)	8 (3%)	1 (0%)	34	66
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%)	34	66

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 ⓘ

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%)	208 (90%)	24 (10%)	7	21
1	D	230/234 (98%)	206 (90%)	24 (10%)	7	21
2	B	93/94 (99%)	86 (92%)	7 (8%)	13	37
2	E	94/94 (100%)	80 (85%)	14 (15%)	3	9
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	7 (88%)	1 (12%)	4	14
All	All	665/672 (99%)	595 (90%)	70 (10%)	6	20

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	24	SER
1	A	45	TYR
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	131	LYS
1	A	137	ASP
1	A	154	GLU
1	A	180	LEU
1	A	181	ARG
1	A	200	THR
1	A	218	GLN
1	A	223	GLU
1	A	228	MET
1	A	234	ARG
1	A	238	ASP

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Mol	Chain	Res	Type
1	A	240	THR
1	A	254	GLU
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	31	LYS
1	D	45	TYR
1	D	53	GLU
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	181	ARG
1	D	196	LYS
1	D	200	THR
1	D	222	GLU
1	D	226	GLN
1	D	227	ASP
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
2	E	48	LYS
2	E	60	TRP

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Mol	Chain	Res	Type
2	E	64	ILE
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	191	HIS

### 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](#)

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	$\# Z  > 2$
5	SO4	A	303	-	4,4,4	0.45	0	6,6,6	0.06	0
4	GOL	A	301	-	5,5,5	0.50	0	5,5,5	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	302	-	5,5,5	1.08	0	5,5,5	2.02	1 (20%)
4	GOL	B	101	-	5,5,5	0.88	0	5,5,5	1.26	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	A	302	-	-	2/4/4/4	-
4	GOL	B	101	-	-	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
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	A	302	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	101	GOL	5	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(Å²)	Q<0.9
1	A	272/276 (98%)	0.31	22 (8%)	12	6	22, 65, 136, 156	16 (5%)
1	D	272/276 (98%)	0.15	8 (2%)	51	41	21, 70, 117, 136	8 (2%)
2	B	97/99 (97%)	-0.25	1 (1%)	82	77	29, 50, 80, 99	0
2	E	99/99 (100%)	-0.23	1 (1%)	82	77	20, 48, 78, 111	0
3	C	9/9 (100%)	-0.25	0	100	100	28, 40, 55, 56	0
3	F	9/9 (100%)	-0.46	0	100	100	12, 34, 61, 64	0
All	All	758/768 (98%)	0.10	32 (4%)	36	26	12, 59, 122, 156	24 (3%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	PRO	6.0
1	A	90	GLY	4.7
1	A	249	VAL	4.6
1	A	256	ASN	4.4
1	A	15	PRO	4.4
1	A	199	VAL	4.3
1	A	89	ALA	4.2
1	D	223	GLU	3.9
1	A	248	VAL	3.7
1	A	187	ALA	3.1
1	A	247	VAL	3.1
1	D	107	TRP	3.0
1	D	17	LEU	2.8
1	A	273	ARG	2.7
2	B	3	LYS	2.6
1	A	250	PRO	2.6
1	A	269	PRO	2.6
1	D	90	GLY	2.5
1	A	230	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	276	PRO	2.4
1	A	255	GLN	2.4
2	E	2	GLN	2.4
1	D	256	ASN	2.3
1	D	16	GLY	2.3
1	A	223	GLU	2.3
1	A	271	THR	2.3
1	A	203	CYS	2.2
1	A	265	GLY	2.1
1	A	270	LEU	2.1
1	A	216	THR	2.1
1	D	181	ARG	2.0
1	A	224	LEU	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 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
5	SO4	A	303	5/5	0.75	0.28	138,139,142,144	0
4	GOL	A	301	6/6	0.90	0.17	33,33,33,34	0
4	GOL	A	302	6/6	0.93	0.19	4,5,5,6	0
4	GOL	B	101	6/6	0.94	0.16	8,9,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.