



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:40 AM GMT

PDB ID : 2NQQ
Title : MoeA R137Q
Authors : Nicolas, J.; Xiang, S.; Schindelin, H.; Rajagopalan, K.V.
Deposited on : 2006-10-31
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

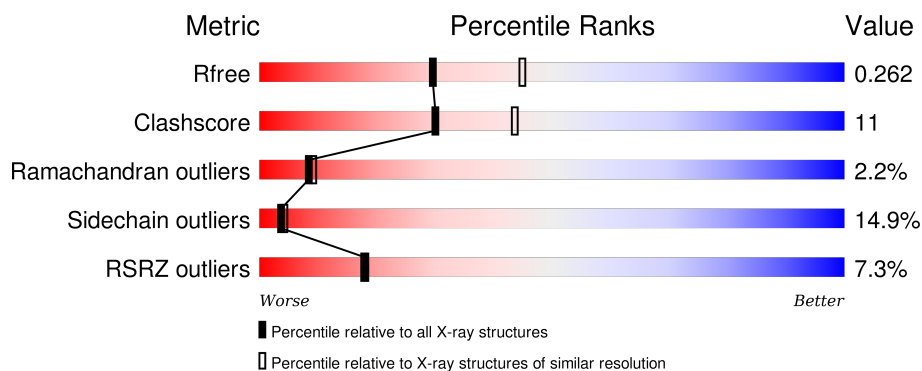
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	411	<div> <div>6%</div> <div>72% 21% 5% .</div> </div>
1	B	411	<div> <div>6%</div> <div>71% 22% 5% .</div> </div>
1	C	411	<div> <div>7%</div> <div>71% 22% . .</div> </div>
1	D	411	<div> <div>14%</div> <div>64% 27% 7% .</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	904	-	-	-	X
2	GOL	A	905	-	-	-	X
2	GOL	A	906	-	-	-	X
2	GOL	B	903	-	-	X	-
2	GOL	B	910	-	-	-	X
2	GOL	C	911	-	-	-	X
2	GOL	D	902	-	-	X	X
2	GOL	D	909	-	-	-	X
2	GOL	D	913	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13077 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.

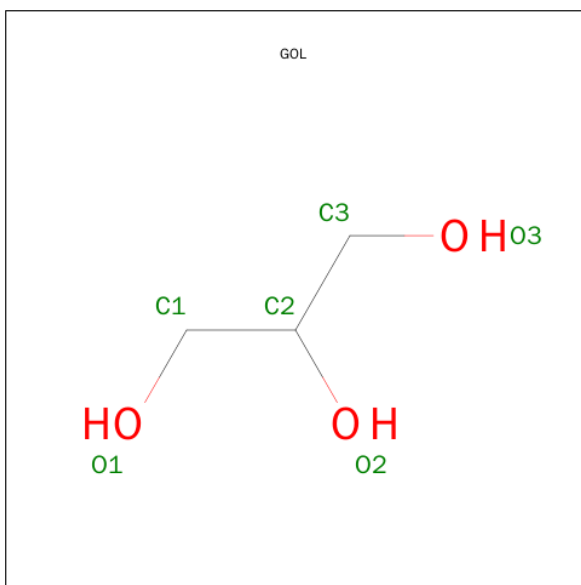
- Molecule 1 is a protein called Molybdopterin biosynthesis protein moeA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3038	1917	529	579	13			
1	B	403	Total	C	N	O	S	0	0	0
			3038	1917	529	579	13			
1	C	403	Total	C	N	O	S	0	0	0
			3038	1917	529	579	13			
1	D	403	Total	C	N	O	S	0	0	0
			3038	1917	529	579	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLN	ARG	ENGINEERED	UNP P12281
B	137	GLN	ARG	ENGINEERED	UNP P12281
C	137	GLN	ARG	ENGINEERED	UNP P12281
D	137	GLN	ARG	ENGINEERED	UNP P12281

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

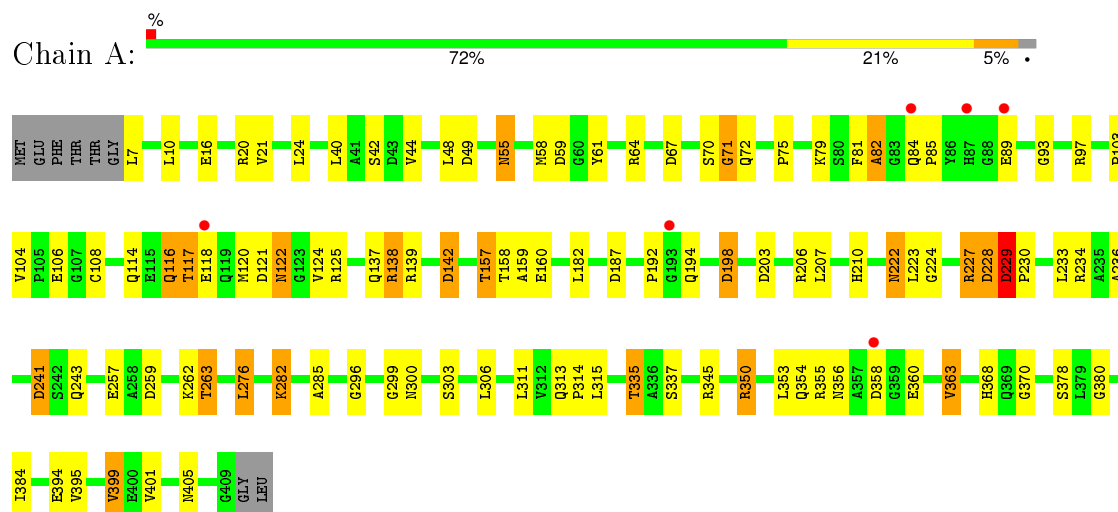
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	249	Total 249	O 249	0	0
3	B	236	Total 236	O 236	0	0
3	C	189	Total 189	O 189	0	0
3	D	167	Total 167	O 167	0	0

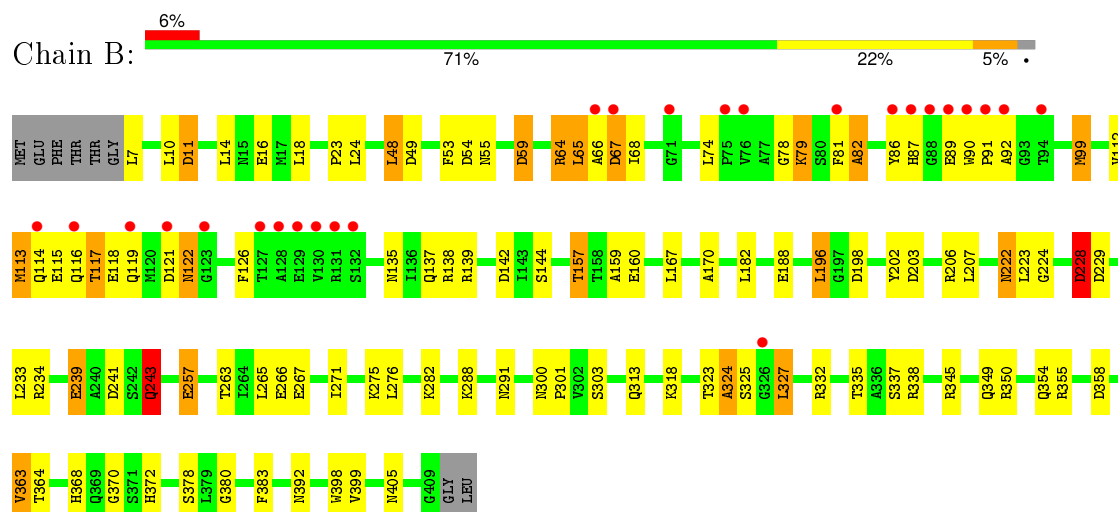
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Molybdopterin biosynthesis protein moeA

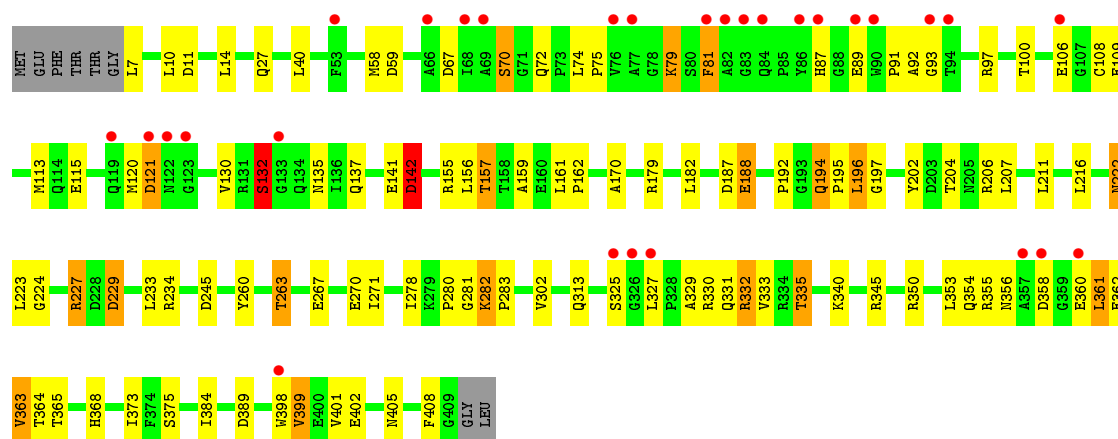


- Molecule 1: Molybdopterin biosynthesis protein moeA

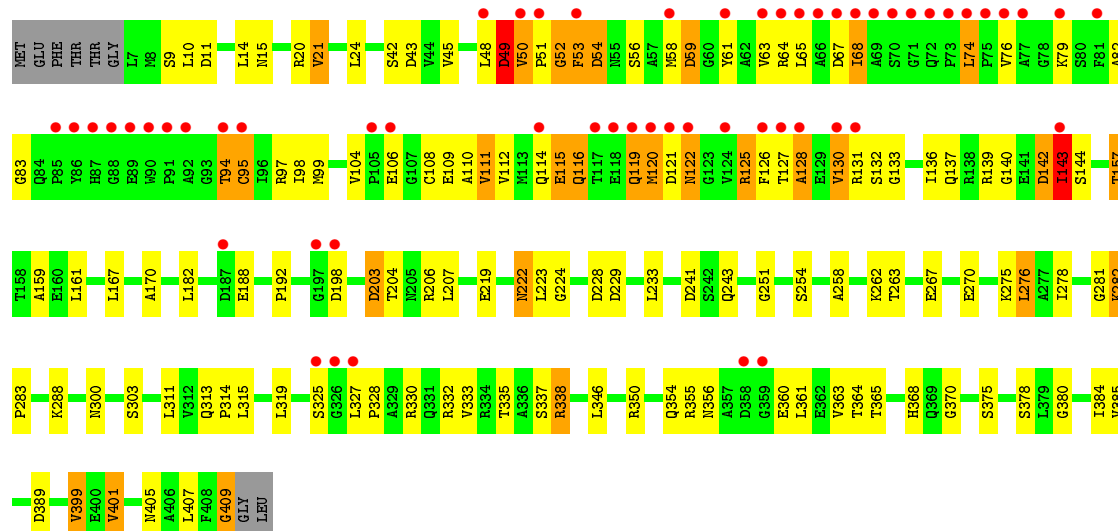


- Molecule 1: Molybdopterin biosynthesis protein moeA





• Molecule 1: Molybdopterin biosynthesis protein moeA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.20Å 106.64Å 99.69Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 47.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (50.00-2.40) 96.9 (47.01-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.190 , 0.261 0.196 , 0.262	Depositor DCC
R_{free} test set	3157 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.6	EDS
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 63637 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13077	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.81	0/3097	0.96	14/4210 (0.3%)
1	B	0.77	1/3097 (0.0%)	0.96	14/4210 (0.3%)
1	C	0.76	0/3097	0.91	9/4210 (0.2%)
1	D	0.77	1/3097 (0.0%)	0.94	11/4210 (0.3%)
All	All	0.78	2/12388 (0.0%)	0.94	48/16840 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	TRP	CB-CG	5.68	1.60	1.50
1	D	399	VAL	CB-CG1	-5.16	1.42	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ASP	CB-CG-OD2	9.21	126.58	118.30
1	A	187	ASP	CB-CG-OD2	9.13	126.52	118.30
1	A	139	ARG	NE-CZ-NH2	-9.09	115.76	120.30
1	B	358	ASP	CB-CG-OD2	8.54	125.99	118.30
1	B	363	VAL	CB-CA-C	-7.88	96.43	111.40
1	B	229	ASP	CB-CG-OD2	7.78	125.31	118.30
1	A	228	ASP	CB-CG-OD2	7.78	125.30	118.30
1	D	11	ASP	CB-CG-OD2	7.70	125.23	118.30
1	A	59	ASP	CB-CG-OD2	7.57	125.12	118.30
1	A	241	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	139	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	121	ASP	CB-CG-OD2	6.70	124.33	118.30
1	D	389	ASP	CB-CG-OD2	6.67	124.30	118.30
1	B	11	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	138	ARG	NE-CZ-NH1	6.18	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	ASP	CB-CG-OD2	6.17	123.85	118.30
1	C	245	ASP	CB-CG-OD2	6.16	123.84	118.30
1	D	241	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	358	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	67	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	363	VAL	CB-CA-C	-5.94	100.12	111.40
1	B	142	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	54	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	234	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	198	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	59	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	345	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	121	ASP	CB-CG-OD2	5.63	123.36	118.30
1	C	59	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	203	ASP	CB-CG-OD2	5.58	123.33	118.30
1	D	409	GLY	CA-C-O	-5.58	110.57	120.60
1	C	67	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	229	ASP	CB-CG-OD2	5.47	123.23	118.30
1	D	49	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	11	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	389	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	229	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	241	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	234	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	142	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	228	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	203	ASP	CB-CG-OD1	5.21	122.98	118.30
1	C	142	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	67	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	121	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	259	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	350	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	B	243	GLN	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3038	0	3032	64	0
1	B	3038	0	3032	72	0
1	C	3038	0	3032	58	0
1	D	3038	0	3032	82	0
2	A	30	0	40	6	0
2	B	18	0	24	9	0
2	C	6	0	8	0	0
2	D	30	0	40	11	0
3	A	249	0	0	16	0
3	B	236	0	0	12	0
3	C	189	0	0	7	0
3	D	167	0	0	13	0
All	All	13077	0	12240	272	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 11.

All (272) 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:B:271:ILE:HG13	3:B:998:HOH:O	1.40	1.17
1:C:142:ASP:OD1	1:C:142:ASP:N	1.89	0.95
1:B:122:ASN:HD22	1:B:122:ASN:H	1.18	0.91
1:A:313:GLN:HE22	1:A:405:ASN:HD21	1.18	0.89
1:D:140:GLY:HA2	1:D:143:ILE:HG23	1.59	0.85
1:C:216:LEU:HD21	1:C:313:GLN:HE21	1.40	0.84
1:D:380:GLY:O	2:D:902:GOL:C3	2.25	0.84
1:A:70:SER:O	1:A:70:SER:OG	1.91	0.83
1:C:282:LYS:HB3	1:C:283:PRO:HD3	1.60	0.82
1:B:243:GLN:OE1	3:B:1106:HOH:O	1.96	0.82
1:D:313:GLN:HE22	1:D:405:ASN:HD21	1.25	0.81
1:D:49:ASP:HA	1:D:143:ILE:HD12	1.60	0.81
1:A:70:SER:C	3:A:1087:HOH:O	2.19	0.80
1:B:368:HIS:HD2	1:B:370:GLY:H	1.26	0.80
1:D:368:HIS:HD2	1:D:370:GLY:H	1.30	0.79
1:C:92:ALA:HA	3:C:1036:HOH:O	1.82	0.79
1:D:222:ASN:HD22	1:D:224:GLY:H	1.31	0.78
1:B:380:GLY:O	2:B:903:GOL:C1	2.31	0.78
1:A:234:ARG:HD2	3:A:1141:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:GLY:O	2:D:902:GOL:H31	1.86	0.76
1:B:300:ASN:HD22	1:B:303:SER:H	1.34	0.76
1:B:368:HIS:CD2	1:B:370:GLY:H	2.04	0.75
1:C:141:GLU:C	1:C:142:ASP:OD1	2.23	0.75
1:A:117:THR:O	1:A:117:THR:HG22	1.88	0.74
1:B:335:THR:HG22	1:B:337:SER:H	1.51	0.74
1:A:70:SER:O	1:A:72:GLN:N	2.19	0.73
1:B:313:GLN:HE22	1:B:405:ASN:HD21	1.34	0.73
1:D:15:ASN:OD1	3:D:1043:HOH:O	2.07	0.72
1:B:257:GLU:OE2	3:B:1045:HOH:O	2.05	0.72
1:A:71:GLY:N	3:A:1087:HOH:O	2.22	0.71
1:D:356:ASN:HD21	1:D:360:GLU:HG3	1.54	0.71
1:D:50:VAL:H	1:D:143:ILE:HG21	1.53	0.71
1:B:380:GLY:O	2:B:903:GOL:H31	1.92	0.70
1:C:7:LEU:N	3:C:1069:HOH:O	2.22	0.70
1:D:328:PRO:CB	3:D:1000:HOH:O	2.39	0.69
1:B:380:GLY:O	2:B:903:GOL:H11	1.92	0.69
1:D:313:GLN:HE22	1:D:405:ASN:ND2	1.91	0.68
1:A:206:ARG:HH11	1:A:222:ASN:HD21	1.41	0.68
1:B:271:ILE:N	1:B:271:ILE:HD12	2.08	0.68
1:D:328:PRO:HB2	3:D:1000:HOH:O	1.93	0.68
1:B:117:THR:HB	3:B:1128:HOH:O	1.94	0.67
1:D:368:HIS:CD2	1:D:370:GLY:H	2.11	0.67
1:C:222:ASN:C	1:C:222:ASN:HD22	1.98	0.67
1:A:300:ASN:HD22	1:A:303:SER:H	1.42	0.65
1:B:378:SER:O	2:B:903:GOL:H32	1.97	0.65
1:A:117:THR:HG23	1:A:124:VAL:CG1	2.27	0.65
1:D:380:GLY:O	2:D:902:GOL:H32	1.96	0.64
1:D:222:ASN:ND2	1:D:224:GLY:H	1.95	0.64
1:A:81:PHE:O	1:A:82:ALA:HB2	1.98	0.64
2:A:908:GOL:H2	3:A:1106:HOH:O	1.97	0.63
1:A:276:LEU:HB2	1:A:282:LYS:O	1.99	0.62
1:A:70:SER:CA	3:A:1087:HOH:O	2.47	0.62
1:C:79:LYS:HZ3	1:C:81:PHE:HE2	1.47	0.62
1:D:335:THR:HG22	1:D:337:SER:H	1.64	0.62
1:D:282:LYS:HB3	1:D:283:PRO:HD3	1.81	0.62
1:B:222:ASN:HD22	1:B:224:GLY:H	1.48	0.62
1:B:243:GLN:CD	3:B:1106:HOH:O	2.36	0.62
1:B:115:GLU:HG3	1:B:116:GLN:N	2.14	0.61
1:B:7:LEU:N	3:B:951:HOH:O	2.33	0.61
1:B:122:ASN:ND2	1:B:122:ASN:H	1.93	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:GLN:HE22	1:C:405:ASN:HD21	1.46	0.61
1:B:122:ASN:HD22	1:B:122:ASN:N	1.90	0.61
1:B:48:LEU:HD11	1:B:167:LEU:HA	1.82	0.61
1:A:137:GLN:HE22	1:A:142:ASP:HB2	1.66	0.61
1:A:368:HIS:HD2	1:A:370:GLY:H	1.49	0.61
1:A:210:HIS:HD2	1:A:222:ASN:OD1	1.82	0.61
1:D:300:ASN:HD22	1:D:303:SER:H	1.48	0.61
1:B:79:LYS:O	1:B:86:TYR:HB2	2.02	0.60
1:D:143:ILE:HG23	1:D:144:SER:H	1.67	0.60
1:A:40:LEU:HD11	1:A:44:VAL:HG23	1.82	0.60
1:B:65:LEU:HG	1:B:66:ALA:H	1.66	0.60
1:B:380:GLY:O	2:B:903:GOL:H12	2.01	0.60
1:C:109:GLU:O	1:C:132:SER:O	2.19	0.59
1:A:21:VAL:HG21	1:A:315:LEU:CD1	2.32	0.59
1:A:313:GLN:HE22	1:A:405:ASN:ND2	1.94	0.59
1:C:202:TYR:O	1:C:204:THR:HG23	2.03	0.59
1:A:299:GLY:O	2:A:904:GOL:H31	2.02	0.58
1:D:378:SER:O	2:D:902:GOL:H31	2.03	0.58
1:A:192:PRO:HB2	1:B:170:ALA:HB2	1.85	0.58
1:D:50:VAL:HB	1:D:51:PRO:HD3	1.85	0.58
1:B:78:GLY:HA3	1:B:86:TYR:CE2	2.39	0.58
1:C:75:PRO:HD2	1:C:93:GLY:O	2.04	0.57
1:B:332:ARG:HG2	1:B:398:TRP:CE3	2.38	0.57
1:B:59:ASP:HB3	1:B:99:MET:HA	1.84	0.57
1:A:122:ASN:H	1:A:122:ASN:HD22	1.51	0.57
1:C:271:ILE:HD12	1:C:271:ILE:N	2.19	0.57
1:A:345:ARG:HD3	3:A:1139:HOH:O	2.02	0.57
1:A:384:ILE:HG23	1:A:399:VAL:CG1	2.35	0.57
1:D:206:ARG:HH11	1:D:222:ASN:HD21	1.51	0.57
1:B:157:THR:HG22	1:B:159:ALA:H	1.70	0.57
1:B:243:GLN:HB3	3:B:1106:HOH:O	2.04	0.56
1:A:157:THR:HG23	1:A:159:ALA:H	1.70	0.56
1:C:373:ILE:HG23	1:D:142:ASP:HB2	1.85	0.56
1:C:27:GLN:NE2	3:C:962:HOH:O	2.18	0.56
1:C:353:LEU:HD13	1:C:363:VAL:HG13	1.87	0.56
1:B:23:PRO:HB2	2:B:910:GOL:H2	1.87	0.56
1:C:192:PRO:HB2	1:D:170:ALA:HB2	1.86	0.56
1:B:313:GLN:HE22	1:B:405:ASN:ND2	2.02	0.55
1:C:330:ARG:NH1	1:C:402:GLU:OE1	2.38	0.55
1:A:75:PRO:HD2	1:A:93:GLY:O	2.07	0.55
1:B:112:VAL:HG11	1:B:116:GLN:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLU:CG	1:B:116:GLN:N	2.69	0.55
1:D:161:LEU:CD1	3:D:1080:HOH:O	2.54	0.55
1:A:229:ASP:HB2	1:A:230:PRO:HD2	1.89	0.55
1:A:117:THR:O	1:A:117:THR:CG2	2.54	0.55
1:A:300:ASN:ND2	1:A:303:SER:H	2.05	0.54
1:C:157:THR:HG22	1:C:159:ALA:H	1.72	0.54
1:B:222:ASN:ND2	1:B:224:GLY:H	2.04	0.54
1:A:263:THR:HB	3:A:997:HOH:O	2.06	0.54
1:A:137:GLN:NE2	1:A:142:ASP:HB2	2.21	0.54
1:C:282:LYS:HB3	1:C:283:PRO:CD	2.36	0.54
1:C:216:LEU:HD21	1:C:313:GLN:NE2	2.17	0.54
1:A:157:THR:HG22	1:A:160:GLU:OE2	2.08	0.54
1:B:114:GLN:HA	3:B:1128:HOH:O	2.08	0.54
1:D:384:ILE:HG23	1:D:399:VAL:CG1	2.38	0.54
1:A:285:ALA:HB3	1:A:296:GLY:HA3	1.90	0.53
2:D:902:GOL:O2	3:D:1029:HOH:O	2.14	0.53
1:C:211:LEU:HD22	3:D:1080:HOH:O	2.07	0.53
1:D:50:VAL:C	1:D:52:GLY:N	2.62	0.53
1:A:157:THR:HG23	1:A:158:THR:N	2.24	0.53
1:B:18:LEU:O	1:B:318:LYS:NZ	2.36	0.53
1:D:222:ASN:HD22	1:D:222:ASN:C	2.12	0.53
1:C:373:ILE:HG23	1:D:142:ASP:CB	2.40	0.52
1:B:81:PHE:O	1:B:82:ALA:CB	2.56	0.52
1:B:288:LYS:NZ	3:B:1066:HOH:O	2.13	0.52
1:B:239:GLU:O	1:B:243:GLN:HG2	2.08	0.52
1:B:368:HIS:CD2	1:B:372:HIS:HE1	2.27	0.52
1:B:275:LYS:HD3	3:B:1012:HOH:O	2.08	0.52
1:A:116:GLN:NE2	3:A:964:HOH:O	2.42	0.52
1:A:81:PHE:O	1:A:82:ALA:CB	2.58	0.52
1:A:21:VAL:HG21	1:A:315:LEU:HD12	1.91	0.52
1:C:281:GLY:O	1:C:282:LYS:HB2	2.09	0.51
1:D:116:GLN:HE21	1:D:116:GLN:N	2.07	0.51
1:B:196:LEU:HD13	1:B:202:TYR:CE2	2.46	0.51
1:D:51:PRO:O	1:D:53:PHE:N	2.43	0.51
1:D:378:SER:O	2:D:902:GOL:C3	2.59	0.51
1:B:49:ASP:OD2	2:B:907:GOL:H31	2.11	0.51
1:A:49:ASP:HB2	2:A:905:GOL:H12	1.92	0.51
1:B:332:ARG:HG2	1:B:398:TRP:HE3	1.76	0.50
1:D:157:THR:HG22	1:D:159:ALA:H	1.74	0.50
1:D:59:ASP:O	1:D:114:GLN:HB2	2.11	0.50
1:C:278:ILE:O	1:C:345:ARG:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:HG13	1:A:108:CYS:HB3	1.92	0.50
1:D:206:ARG:HD2	1:D:222:ASN:HD21	1.76	0.50
1:D:51:PRO:HB2	1:D:139:ARG:HA	1.93	0.50
1:D:281:GLY:O	1:D:282:LYS:HB2	2.11	0.50
1:A:236:ALA:HB2	2:A:906:GOL:H11	1.93	0.49
1:A:243:GLN:NE2	3:A:953:HOH:O	2.28	0.49
1:B:323:THR:C	1:B:324:ALA:O	2.51	0.49
1:A:313:GLN:HB3	1:A:314:PRO:HD3	1.95	0.49
1:B:81:PHE:O	1:B:82:ALA:HB3	2.13	0.49
1:A:257:GLU:HG3	3:A:1156:HOH:O	2.11	0.49
1:A:356:ASN:HD21	1:A:360:GLU:CB	2.25	0.49
1:A:353:LEU:HD13	1:A:401:VAL:HG11	1.94	0.49
1:D:328:PRO:HD3	3:D:969:HOH:O	2.13	0.49
1:C:333:VAL:CG1	1:C:362:GLU:HA	2.43	0.49
1:D:258:ALA:HA	1:D:262:LYS:HD3	1.95	0.49
1:D:251:GLY:HA3	2:D:912:GOL:O1	2.13	0.48
1:D:51:PRO:HD2	1:D:143:ILE:HG22	1.96	0.48
1:C:58:MET:HA	1:C:100:THR:OG1	2.13	0.48
1:D:300:ASN:ND2	1:D:303:SER:H	2.11	0.48
1:D:68:ILE:O	1:D:68:ILE:HD13	2.13	0.48
1:A:380:GLY:O	3:A:909:HOH:O	2.20	0.48
1:C:142:ASP:CG	3:C:1002:HOH:O	2.50	0.48
1:A:335:THR:HG22	1:A:337:SER:H	1.78	0.48
1:B:206:ARG:HD2	1:B:222:ASN:HD21	1.78	0.48
1:B:65:LEU:HD12	1:B:66:ALA:HB2	1.96	0.48
1:A:222:ASN:HD22	1:A:224:GLY:H	1.62	0.48
1:B:116:GLN:O	1:B:126:PHE:HA	2.14	0.48
1:A:368:HIS:CD2	1:A:370:GLY:H	2.30	0.48
1:A:276:LEU:HD21	1:A:311:LEU:HD11	1.96	0.47
1:D:355:ARG:O	3:D:1046:HOH:O	2.20	0.47
1:C:206:ARG:HH11	1:C:222:ASN:HD21	1.62	0.47
1:C:170:ALA:HB2	1:D:192:PRO:HB2	1.96	0.47
1:D:74:LEU:HB3	1:D:94:THR:HA	1.97	0.47
1:B:300:ASN:ND2	1:B:303:SER:H	2.07	0.47
1:D:276:LEU:HD21	1:D:311:LEU:HD11	1.96	0.47
1:B:222:ASN:HD22	1:B:222:ASN:C	2.17	0.47
1:A:55:ASN:ND2	1:A:137:GLN:HB3	2.30	0.47
1:D:125:ARG:HA	1:D:125:ARG:NE	2.30	0.47
1:B:239:GLU:OE2	1:B:243:GLN:NE2	2.47	0.46
1:A:118:GLU:O	1:A:125:ARG:HB3	2.15	0.46
1:D:104:VAL:HG21	1:D:136:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ILE:HG23	1:D:399:VAL:HG11	1.98	0.46
1:D:409:GLY:HA2	2:D:909:GOL:H12	1.96	0.46
1:D:49:ASP:HB2	1:D:52:GLY:HA2	1.98	0.46
1:D:363:VAL:HG21	1:D:401:VAL:HG21	1.97	0.46
1:B:378:SER:O	2:B:903:GOL:C3	2.64	0.45
1:C:58:MET:SD	1:C:135:ASN:ND2	2.89	0.45
1:B:65:LEU:HG	1:B:66:ALA:N	2.31	0.45
1:B:49:ASP:OD1	2:B:907:GOL:H12	2.16	0.45
1:A:85:PRO:HB3	1:A:103:PRO:HG2	1.97	0.45
1:D:133:GLY:O	1:D:136:ILE:HG13	2.16	0.45
1:C:280:PRO:HG3	1:C:302:VAL:HG12	1.99	0.45
1:D:51:PRO:HD3	1:D:142:ASP:OD2	2.16	0.45
1:A:70:SER:HA	3:A:1087:HOH:O	2.12	0.45
1:B:157:THR:HB	1:B:160:GLU:OE2	2.16	0.45
1:A:64:ARG:NH1	1:A:67:ASP:OD1	2.49	0.45
1:D:405:ASN:OD1	1:D:407:LEU:HG	2.17	0.45
1:C:75:PRO:CD	1:C:93:GLY:O	2.64	0.45
1:D:203:ASP:OD1	2:D:912:GOL:O3	2.35	0.45
1:A:394:GLU:O	1:A:395:VAL:C	2.53	0.45
1:C:222:ASN:ND2	1:C:224:GLY:H	2.14	0.45
1:C:113:MET:HE3	1:C:115:GLU:OE1	2.16	0.45
1:A:61:TYR:CE1	1:A:117:THR:HG21	2.52	0.44
1:A:55:ASN:HD21	1:A:137:GLN:HB3	1.81	0.44
1:B:74:LEU:HD12	1:B:126:PHE:CE1	2.53	0.44
1:B:338:ARG:HH22	1:B:392:ASN:HD22	1.63	0.44
1:D:127:THR:O	1:D:128:ALA:C	2.55	0.44
1:B:349:GLN:O	1:B:383:PHE:HA	2.17	0.44
1:B:198:ASP:N	3:B:1064:HOH:O	2.49	0.44
1:D:364:THR:HG22	1:D:365:THR:O	2.17	0.44
1:B:113:MET:CE	1:B:135:ASN:HD21	2.31	0.44
1:C:194:GLN:HG3	1:C:195:PRO:HD2	1.99	0.44
1:B:53:PHE:O	1:B:54:ASP:C	2.56	0.44
1:D:319:LEU:HD23	1:D:319:LEU:HA	1.83	0.44
1:D:161:LEU:HD13	3:D:1080:HOH:O	2.15	0.43
1:C:384:ILE:HG23	1:C:399:VAL:CG1	2.48	0.43
3:A:1131:HOH:O	1:B:332:ARG:HD2	2.17	0.43
1:D:56:SER:OG	1:D:111:VAL:HG11	2.17	0.43
1:C:260:TYR:HA	1:C:263:THR:HG23	2.00	0.43
1:C:332:ARG:HG2	1:C:398:TRP:CE3	2.53	0.43
1:D:330:ARG:NH1	1:D:385:VAL:HG11	2.34	0.43
1:D:115:GLU:C	1:D:116:GLN:HE21	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:VAL:CG1	1:D:363:VAL:HG23	2.49	0.43
1:C:40:LEU:HG	1:C:156:LEU:HD21	2.01	0.43
1:B:206:ARG:HH11	1:B:222:ASN:HD21	1.66	0.43
1:C:363:VAL:HG11	1:C:401:VAL:HG21	2.00	0.43
1:C:188:GLU:HG2	1:D:82:ALA:HB1	2.01	0.43
1:C:375:SER:HA	3:C:918:HOH:O	2.19	0.43
1:A:384:ILE:HG23	1:A:399:VAL:HG11	2.00	0.42
1:C:227:ARG:O	1:C:229:ASP:N	2.52	0.42
1:C:408:PHE:HA	1:D:157:THR:HG23	2.01	0.42
1:D:276:LEU:HB3	1:D:278:ILE:HG12	2.00	0.42
1:A:203:ASP:OD1	2:A:904:GOL:H11	2.19	0.42
1:C:333:VAL:HG13	1:C:362:GLU:HA	2.02	0.42
1:C:155:ARG:HH12	2:D:909:GOL:C1	2.32	0.42
1:C:157:THR:CG2	1:C:159:ALA:H	2.31	0.42
1:B:122:ASN:N	1:B:122:ASN:ND2	2.61	0.42
1:D:119:GLN:O	1:D:120:MET:CB	2.68	0.42
1:C:333:VAL:HG13	1:C:361:LEU:O	2.20	0.42
1:C:222:ASN:C	1:C:222:ASN:ND2	2.71	0.41
1:D:61:TYR:CD2	1:D:95:CYS:SG	3.14	0.41
1:B:64:ARG:HB2	1:B:67:ASP:OD2	2.20	0.41
1:D:375:SER:HA	3:D:920:HOH:O	2.19	0.41
1:B:265:LEU:HD22	1:B:271:ILE:HG12	2.02	0.41
1:D:281:GLY:HA2	1:D:303:SER:HB3	2.02	0.41
1:C:364:THR:HG22	1:C:365:THR:O	2.20	0.41
1:D:338:ARG:O	2:D:913:GOL:H32	2.20	0.41
1:A:227:ARG:NE	3:A:1116:HOH:O	2.54	0.41
1:D:112:VAL:HG22	1:D:130:VAL:HG12	2.03	0.41
1:C:222:ASN:HD22	1:C:224:GLY:H	1.69	0.41
1:D:53:PHE:HB2	3:D:1075:HOH:O	2.21	0.41
1:A:345:ARG:CD	3:A:1139:HOH:O	2.63	0.41
2:A:908:GOL:C3	3:A:983:HOH:O	2.68	0.41
1:C:196:LEU:HD13	1:C:202:TYR:CZ	2.55	0.41
1:D:56:SER:HB2	1:D:98:ILE:HD13	2.03	0.41
1:D:346:LEU:HD13	3:D:947:HOH:O	2.19	0.41
1:D:313:GLN:HB3	1:D:314:PRO:HD3	2.02	0.41
1:D:21:VAL:HG21	1:D:315:LEU:HD11	2.03	0.41
1:C:335:THR:HA	1:C:363:VAL:HG23	2.03	0.40
1:C:161:LEU:N	1:C:162:PRO:CD	2.84	0.40
1:C:179:ARG:HD3	3:C:1082:HOH:O	2.21	0.40
1:C:356:ASN:HD21	1:C:360:GLU:HG2	1.86	0.40
1:C:234:ARG:NH2	3:C:1087:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:ILE:HG12	3:D:1004:HOH:O	2.21	0.40
1:B:87:HIS:HB2	3:B:1051:HOH:O	2.22	0.40
1:D:50:VAL:O	1:D:52:GLY:N	2.55	0.40
1:A:61:TYR:CD1	1:A:117:THR:HG21	2.56	0.40
1:A:21:VAL:HG21	1:A:315:LEU:HD11	2.04	0.40
1:B:300:ASN:HA	1:B:301:PRO:HD3	1.95	0.40
1:B:55:ASN:OD1	1:B:137:GLN:HB3	2.21	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	401/411 (98%)	385 (96%)	11 (3%)	5 (1%)	16	23
1	B	401/411 (98%)	378 (94%)	16 (4%)	7 (2%)	11	14
1	C	401/411 (98%)	364 (91%)	31 (8%)	6 (2%)	13	17
1	D	401/411 (98%)	356 (89%)	28 (7%)	17 (4%)	3	2
All	All	1604/1644 (98%)	1483 (92%)	86 (5%)	35 (2%)	8	9

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
1	A	228	ASP
1	A	282	LYS
1	B	82	ALA
1	B	91	PRO
1	B	324	ALA
1	C	91	PRO
1	C	282	LYS

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Mol	Chain	Res	Type
1	D	52	GLY
1	D	120	MET
1	D	122	ASN
1	D	128	ALA
1	D	282	LYS
1	A	71	GLY
1	B	92	ALA
1	B	228	ASP
1	B	282	LYS
1	C	70	SER
1	C	197	GLY
1	D	63	VAL
1	D	111	VAL
1	D	121	ASP
1	C	132	SER
1	D	50	VAL
1	D	325	SER
1	A	198	ASP
1	C	329	ALA
1	D	43	ASP
1	D	54	ASP
1	D	110	ALA
1	D	130	VAL
1	B	327	LEU
1	D	143	ILE
1	D	76	VAL
1	D	83	GLY

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	325/331 (98%)	283 (87%)	42 (13%)	5	6
1	B	325/331 (98%)	279 (86%)	46 (14%)	4	4
1	C	325/331 (98%)	280 (86%)	45 (14%)	4	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	325/331 (98%)	264 (81%)	61 (19%)	2	2
All	All	1300/1324 (98%)	1106 (85%)	194 (15%)	4	4

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	10	LEU
1	A	16	GLU
1	A	20	ARG
1	A	24	LEU
1	A	42	SER
1	A	48	LEU
1	A	55	ASN
1	A	58	MET
1	A	79	LYS
1	A	84	GLN
1	A	89	GLU
1	A	97	ARG
1	A	106	GLU
1	A	114	GLN
1	A	116	GLN
1	A	117	THR
1	A	120	MET
1	A	122	ASN
1	A	138	ARG
1	A	157	THR
1	A	182	LEU
1	A	194	GLN
1	A	207	LEU
1	A	222	ASN
1	A	223	LEU
1	A	227	ARG
1	A	229	ASP
1	A	233	LEU
1	A	241	ASP
1	A	262	LYS
1	A	263	THR
1	A	276	LEU
1	A	306	LEU
1	A	335	THR
1	A	350	ARG

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Mol	Chain	Res	Type
1	A	354	GLN
1	A	355	ARG
1	A	358	ASP
1	A	363	VAL
1	A	378	SER
1	A	399	VAL
1	B	10	LEU
1	B	11	ASP
1	B	14	LEU
1	B	16	GLU
1	B	24	LEU
1	B	48	LEU
1	B	59	ASP
1	B	64	ARG
1	B	65	LEU
1	B	68	ILE
1	B	79	LYS
1	B	89	GLU
1	B	99	MET
1	B	113	MET
1	B	117	THR
1	B	118	GLU
1	B	119	GLN
1	B	122	ASN
1	B	138	ARG
1	B	139	ARG
1	B	144	SER
1	B	157	THR
1	B	182	LEU
1	B	188	GLU
1	B	196	LEU
1	B	207	LEU
1	B	222	ASN
1	B	223	LEU
1	B	228	ASP
1	B	233	LEU
1	B	239	GLU
1	B	243	GLN
1	B	257	GLU
1	B	263	THR
1	B	266	GLU
1	B	267	GLU

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Mol	Chain	Res	Type
1	B	276	LEU
1	B	291	ASN
1	B	325	SER
1	B	327	LEU
1	B	350	ARG
1	B	354	GLN
1	B	355	ARG
1	B	363	VAL
1	B	364	THR
1	B	399	VAL
1	C	10	LEU
1	C	14	LEU
1	C	70	SER
1	C	72	GLN
1	C	74	LEU
1	C	79	LYS
1	C	81	PHE
1	C	87	HIS
1	C	89	GLU
1	C	97	ARG
1	C	106	GLU
1	C	108	CYS
1	C	120	MET
1	C	121	ASP
1	C	130	VAL
1	C	132	SER
1	C	137	GLN
1	C	142	ASP
1	C	157	THR
1	C	182	LEU
1	C	187	ASP
1	C	188	GLU
1	C	194	GLN
1	C	196	LEU
1	C	207	LEU
1	C	222	ASN
1	C	223	LEU
1	C	227	ARG
1	C	233	LEU
1	C	263	THR
1	C	267	GLU
1	C	270	GLU

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Mol	Chain	Res	Type
1	C	325	SER
1	C	327	LEU
1	C	331	GLN
1	C	332	ARG
1	C	335	THR
1	C	340	LYS
1	C	350	ARG
1	C	354	GLN
1	C	355	ARG
1	C	361	LEU
1	C	363	VAL
1	C	368	HIS
1	C	399	VAL
1	D	9	SER
1	D	10	LEU
1	D	14	LEU
1	D	20	ARG
1	D	21	VAL
1	D	24	LEU
1	D	42	SER
1	D	45	VAL
1	D	48	LEU
1	D	49	ASP
1	D	53	PHE
1	D	58	MET
1	D	64	ARG
1	D	65	LEU
1	D	68	ILE
1	D	74	LEU
1	D	79	LYS
1	D	94	THR
1	D	95	CYS
1	D	97	ARG
1	D	99	MET
1	D	106	GLU
1	D	108	CYS
1	D	109	GLU
1	D	115	GLU
1	D	116	GLN
1	D	119	GLN
1	D	122	ASN
1	D	125	ARG

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Mol	Chain	Res	Type
1	D	126	PHE
1	D	131	ARG
1	D	132	SER
1	D	137	GLN
1	D	142	ASP
1	D	143	ILE
1	D	157	THR
1	D	167	LEU
1	D	182	LEU
1	D	188	GLU
1	D	198	ASP
1	D	204	THR
1	D	207	LEU
1	D	219	GLU
1	D	222	ASN
1	D	223	LEU
1	D	233	LEU
1	D	243	GLN
1	D	254	SER
1	D	263	THR
1	D	267	GLU
1	D	270	GLU
1	D	275	LYS
1	D	276	LEU
1	D	288	LYS
1	D	327	LEU
1	D	332	ARG
1	D	338	ARG
1	D	350	ARG
1	D	354	GLN
1	D	361	LEU
1	D	401	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	55	ASN
1	A	116	GLN
1	A	122	ASN
1	A	137	GLN
1	A	210	HIS

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Mol	Chain	Res	Type
1	A	222	ASN
1	A	300	ASN
1	A	313	GLN
1	A	331	GLN
1	A	368	HIS
1	B	15	ASN
1	B	116	GLN
1	B	122	ASN
1	B	135	ASN
1	B	190	GLN
1	B	194	GLN
1	B	210	HIS
1	B	222	ASN
1	B	300	ASN
1	B	313	GLN
1	B	368	HIS
1	C	135	ASN
1	C	210	HIS
1	C	222	ASN
1	C	300	ASN
1	C	313	GLN
1	C	354	GLN
1	D	15	ASN
1	D	55	ASN
1	D	116	GLN
1	D	119	GLN
1	D	194	GLN
1	D	210	HIS
1	D	222	ASN
1	D	300	ASN
1	D	313	GLN
1	D	368	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
2	GOL	A	901	-	5,5,5	0.61	0	5,5,5	0.52	0
2	GOL	A	904	-	5,5,5	0.33	0	5,5,5	0.84	0
2	GOL	A	905	-	5,5,5	0.50	0	5,5,5	1.11	0
2	GOL	A	906	-	5,5,5	0.58	0	5,5,5	0.86	0
2	GOL	A	908	-	5,5,5	0.48	0	5,5,5	0.62	0
2	GOL	B	903	-	5,5,5	0.36	0	5,5,5	1.22	1 (20%)
2	GOL	B	907	-	5,5,5	0.40	0	5,5,5	0.27	0
2	GOL	B	910	-	5,5,5	0.59	0	5,5,5	0.77	0
2	GOL	C	911	-	5,5,5	0.39	0	5,5,5	0.31	0
2	GOL	D	902	-	5,5,5	0.77	0	5,5,5	0.69	0
2	GOL	D	909	-	5,5,5	0.65	0	5,5,5	1.07	0
2	GOL	D	912	-	5,5,5	0.38	0	5,5,5	0.40	0
2	GOL	D	913	-	5,5,5	0.34	0	5,5,5	0.58	0
2	GOL	D	914	-	5,5,5	0.28	0	5,5,5	0.34	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
2	GOL	A	901	-	-	0/4/4/4	0/0/0/0
2	GOL	A	904	-	-	0/4/4/4	0/0/0/0
2	GOL	A	905	-	-	0/4/4/4	0/0/0/0
2	GOL	A	906	-	-	0/4/4/4	0/0/0/0
2	GOL	A	908	-	-	0/4/4/4	0/0/0/0
2	GOL	B	903	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	907	-	-	0/4/4/4	0/0/0/0
2	GOL	B	910	-	-	0/4/4/4	0/0/0/0
2	GOL	C	911	-	-	0/4/4/4	0/0/0/0
2	GOL	D	902	-	-	0/4/4/4	0/0/0/0
2	GOL	D	909	-	-	0/4/4/4	0/0/0/0
2	GOL	D	912	-	-	0/4/4/4	0/0/0/0
2	GOL	D	913	-	-	0/4/4/4	0/0/0/0
2	GOL	D	914	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	903	GOL	O1-C1-C2	2.12	120.47	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	904	GOL	2	0
2	A	905	GOL	1	0
2	A	906	GOL	1	0
2	A	908	GOL	2	0
2	B	903	GOL	6	0
2	B	907	GOL	2	0
2	B	910	GOL	1	0
2	D	902	GOL	6	0
2	D	909	GOL	2	0
2	D	912	GOL	2	0
2	D	913	GOL	1	0

5.7 Other polymers

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	403/411 (98%)	-0.22	6 (1%) 76 75	18, 32, 59, 83	0
1	B	403/411 (98%)	0.11	26 (6%) 22 22	20, 34, 83, 107	0
1	C	403/411 (98%)	0.07	29 (7%) 18 18	22, 38, 75, 90	0
1	D	403/411 (98%)	0.51	57 (14%) 4 4	21, 38, 105, 115	0
All	All	1612/1644 (98%)	0.12	118 (7%) 18 18	18, 35, 84, 115	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	66	ALA	14.2
1	D	325	SER	9.8
1	B	130	VAL	9.5
1	D	65	LEU	8.7
1	B	90	TRP	8.6
1	B	131	ARG	8.2
1	C	327	LEU	7.1
1	D	67	ASP	7.1
1	D	69	ALA	6.8
1	C	83	GLY	6.6
1	D	71	GLY	6.5
1	B	116	GLN	6.2
1	D	127	THR	6.1
1	B	89	GLU	6.0
1	D	327	LEU	5.9
1	D	86	TYR	5.5
1	D	120	MET	5.2
1	D	92	ALA	5.1
1	D	88	GLY	5.0
1	C	87	HIS	4.7
1	D	124	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	326	GLY	4.6
1	D	70	SER	4.6
1	D	74	LEU	4.6
1	D	72	GLN	4.5
1	D	126	PHE	4.5
1	D	119	GLN	4.4
1	D	75	PRO	4.2
1	D	94	THR	4.2
1	B	88	GLY	4.1
1	D	121	ASP	4.0
1	D	128	ALA	4.0
1	D	73	PRO	3.9
1	D	50	VAL	3.9
1	D	130	VAL	3.8
1	B	87	HIS	3.8
1	C	357	ALA	3.7
1	D	87	HIS	3.7
1	C	66	ALA	3.7
1	B	128	ALA	3.6
1	A	358	ASP	3.6
1	D	58	MET	3.6
1	C	121	ASP	3.6
1	B	127	THR	3.6
1	D	118	GLU	3.6
1	C	81	PHE	3.5
1	C	82	ALA	3.5
1	C	76	VAL	3.5
1	C	94	THR	3.4
1	D	89	GLU	3.4
1	D	90	TRP	3.3
1	B	119	GLN	3.2
1	D	326	GLY	3.2
1	C	325	SER	3.2
1	B	121	ASP	3.1
1	D	91	PRO	3.1
1	B	67	ASP	3.1
1	D	131	ARG	3.0
1	D	68	ILE	3.0
1	C	358	ASP	3.0
1	D	358	ASP	3.0
1	B	92	ALA	3.0
1	B	81	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	89	GLU	3.0
1	B	66	ALA	3.0
1	D	79	LYS	2.9
1	D	51	PRO	2.9
1	C	123	GLY	2.9
1	D	63	VAL	2.9
1	D	76	VAL	2.9
1	D	53	PHE	2.8
1	D	197	GLY	2.8
1	C	90	TRP	2.8
1	D	198	ASP	2.7
1	B	114	GLN	2.7
1	B	91	PRO	2.7
1	C	89	GLU	2.7
1	C	53	PHE	2.6
1	D	61	TYR	2.6
1	C	68	ILE	2.6
1	A	193	GLY	2.6
1	B	94	THR	2.5
1	B	123	GLY	2.5
1	C	122	ASN	2.5
1	B	129	GLU	2.5
1	C	93	GLY	2.5
1	C	84	GLN	2.5
1	D	143	ILE	2.5
1	C	106	GLU	2.5
1	A	84	GLN	2.4
1	D	122	ASN	2.4
1	D	48	LEU	2.4
1	B	132	SER	2.3
1	D	77	ALA	2.3
1	C	86	TYR	2.3
1	B	86	TYR	2.3
1	D	64	ARG	2.3
1	D	95	CYS	2.3
1	C	360	GLU	2.2
1	D	106	GLU	2.2
1	D	114	GLN	2.2
1	B	71	GLY	2.2
1	B	76	VAL	2.2
1	A	118	GLU	2.2
1	C	398	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	69	ALA	2.1
1	D	359	GLY	2.1
1	C	119	GLN	2.1
1	D	117	THR	2.1
1	C	77	ALA	2.1
1	D	81	PHE	2.1
1	B	326	GLY	2.1
1	D	105	PRO	2.1
1	D	187	ASP	2.1
1	A	87	HIS	2.1
1	D	85	PRO	2.1
1	C	133	GLY	2.0
1	B	75	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	905	6/6	0.77	0.40	17.06	37,47,49,50	0
2	GOL	C	911	6/6	0.87	0.24	7.29	55,57,57,59	0
2	GOL	A	906	6/6	0.84	0.31	6.49	47,50,52,52	0
2	GOL	B	910	6/6	0.88	0.19	5.66	46,48,50,50	0
2	GOL	D	909	6/6	0.87	0.17	4.83	37,44,49,53	0
2	GOL	D	913	6/6	0.89	0.29	4.52	46,51,54,56	0
2	GOL	D	902	6/6	0.82	0.17	4.02	28,37,40,41	0
2	GOL	A	904	6/6	0.89	0.19	3.87	28,36,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	D	912	6/6	0.90	0.16	2.00	41,43,45,48	0
2	GOL	B	907	6/6	0.89	0.18	1.37	46,49,52,52	0
2	GOL	B	903	6/6	0.92	0.14	0.33	26,33,38,39	0
2	GOL	A	901	6/6	0.73	0.17	-0.13	42,52,54,56	0
2	GOL	A	908	6/6	0.90	0.13	-0.38	33,38,39,41	0
2	GOL	D	914	6/6	0.83	0.22	-	63,65,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.