



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:48 AM UTC

PDB ID : 1NRK / pdb_00001nrk
Title : YGFZ PROTEIN
Authors : Teplyakov, A.; Obmolova, G.; Gilliland, G.L.; Structure 2 Function Project (S2F)
Deposited on : 2003-01-24
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

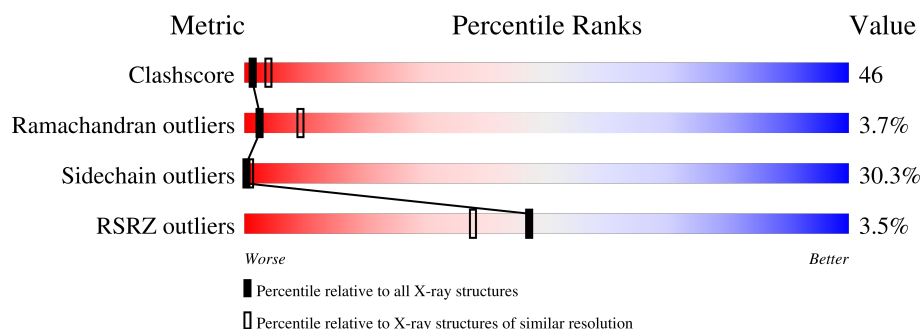
1 Overall quality at a glance

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))
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	328	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2761 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 YGFZ Protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	Se	0	1	0
			2536	1600	445	479	2	10			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P39179
A	-1	SER	-	expression tag	UNP P39179
A	0	HIS	-	expression tag	UNP P39179
A	1	MSE	MET	modified residue	UNP P39179
A	22	MSE	MET	modified residue	UNP P39179
A	41	MSE	MET	modified residue	UNP P39179
A	52	MSE	MET	modified residue	UNP P39179
A	69	MSE	MET	modified residue	UNP P39179
A	172	MSE	MET	modified residue	UNP P39179
A	234	MSE	MET	modified residue	UNP P39179
A	269	MSE	MET	modified residue	UNP P39179
A	296	MSE	MET	modified residue	UNP P39179
A	300	MSE	MET	modified residue	UNP P39179

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

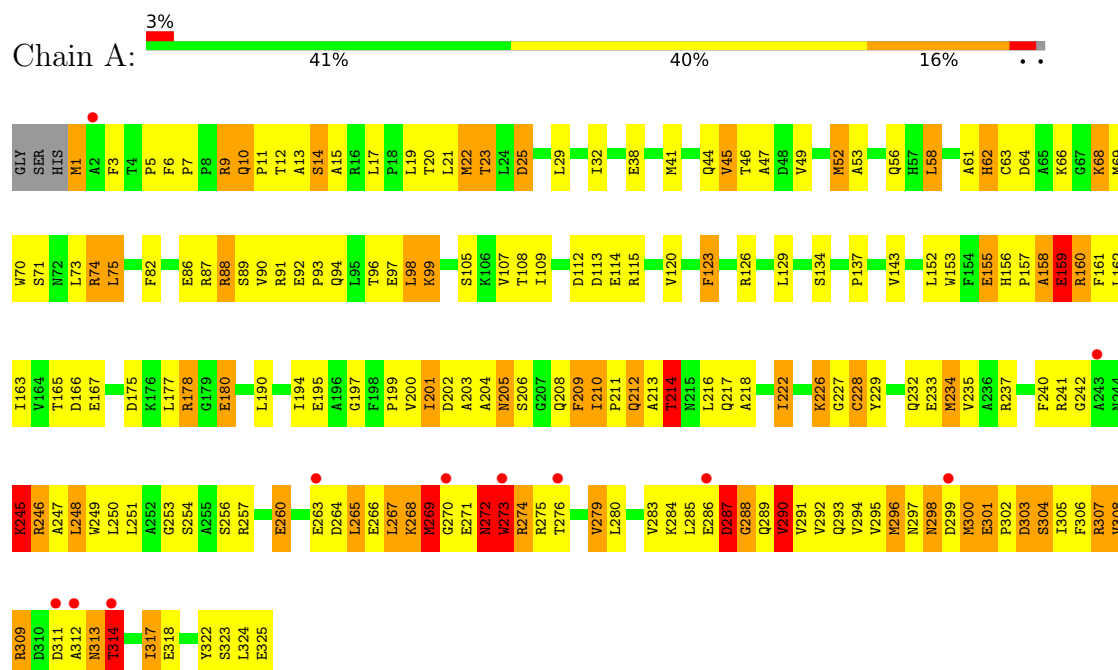
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	215	Total	O	0	0
			215	215		

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: YGFZ Protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.00Å 151.00Å 68.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.80) 92.2 (10.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.193 , 0.252 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2761	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.75	0/2582	1.13	14/3483 (0.4%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	GLY	N-CA-C	-9.88	101.02	114.95
1	A	123	PHE	CA-C-N	-7.31	107.58	121.54
1	A	123	PHE	C-N-CA	-7.31	107.58	121.54
1	A	166	ASP	CB-CA-C	-6.17	96.89	109.65
1	A	272	ASN	N-CA-C	5.93	118.42	109.41
1	A	209	PHE	N-CA-C	5.85	118.74	109.50
1	A	63	CYS	N-CA-C	5.52	118.25	110.14
1	A	290	VAL	CB-CA-C	-5.20	104.07	111.19
1	A	165	THR	CA-C-N	5.20	129.65	120.87
1	A	165	THR	C-N-CA	5.20	129.65	120.87
1	A	9[A]	ARG	N-CA-C	-5.14	101.26	109.23
1	A	9[B]	ARG	N-CA-C	-5.14	101.26	109.23
1	A	214	THR	N-CA-C	-5.07	106.66	114.16
1	A	165	THR	N-CA-C	5.06	115.21	108.38

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	2536	0	2525	231	0
2	A	10	0	0	1	0
3	A	215	0	0	11	0
All	All	2761	0	2525	231	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 46.

All (231) 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:A:299:ASP:O	1:A:300:MSE:HG2	1.13	1.26
1:A:269:MSE:O	1:A:269:MSE:HG2	1.42	1.18
1:A:276:THR:HG21	1:A:300:MSE:HE1	1.12	1.11
1:A:52:MSE:CE	1:A:58:LEU:HD11	1.79	1.11
1:A:267:LEU:HD22	1:A:268:LYS:H	0.93	1.08
1:A:52:MSE:HE2	1:A:58:LEU:HD11	1.33	1.06
1:A:299:ASP:O	1:A:300:MSE:CG	2.05	1.04
1:A:62:HIS:CE1	1:A:70:TRP:HD1	1.75	1.03
1:A:266:GLU:OE2	1:A:309:ARG:HG2	1.58	1.03
1:A:234:MSE:HG2	1:A:237:ARG:NH2	1.73	1.03
1:A:52:MSE:CE	1:A:58:LEU:CD1	2.38	1.02
1:A:86:GLU:OE1	1:A:94:GLN:NE2	1.94	1.00
1:A:158:ALA:O	1:A:159:GLU:HB3	1.60	1.00
1:A:267:LEU:HD22	1:A:268:LYS:N	1.78	0.98
1:A:314:THR:HG22	1:A:314:THR:O	1.61	0.97
1:A:226:LYS:HD2	1:A:227:GLY:H	1.29	0.96
1:A:267:LEU:CD2	1:A:268:LYS:H	1.79	0.96
1:A:52:MSE:HE1	1:A:58:LEU:HD13	1.50	0.94
1:A:287:ASP:HB2	1:A:289:GLN:HG2	1.49	0.94
1:A:276:THR:CG2	1:A:300:MSE:HE1	1.98	0.93
1:A:276:THR:HG21	1:A:300:MSE:CE	1.99	0.93
1:A:287:ASP:CB	1:A:289:GLN:HG2	1.99	0.93
1:A:301:GLU:O	1:A:303:ASP:N	2.02	0.93
1:A:66:LYS:O	1:A:234:MSE:HG3	1.70	0.91
1:A:204:ALA:C	1:A:205:ASN:HD22	1.79	0.90
1:A:205:ASN:HD22	1:A:205:ASN:N	1.66	0.89
1:A:23:THR:HG23	1:A:25:ASP:OD1	1.72	0.88
1:A:268:LYS:HG3	1:A:305:ILE:HB	1.57	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:CD	1:A:227:GLY:H	1.89	0.85
1:A:70:TRP:O	1:A:206:SER:HB2	1.76	0.85
1:A:264:ASP:HB2	1:A:309:ARG:HG3	1.59	0.85
1:A:52:MSE:HE1	1:A:58:LEU:CD1	2.04	0.84
1:A:155:GLU:HG2	1:A:156:HIS:CE1	2.11	0.84
1:A:299:ASP:C	1:A:300:MSE:HG2	2.02	0.84
1:A:226:LYS:HD2	1:A:227:GLY:N	1.91	0.83
1:A:62:HIS:CE1	1:A:70:TRP:CD1	2.66	0.82
1:A:280:LEU:HB2	1:A:293:GLN:HG2	1.61	0.82
1:A:266:GLU:O	1:A:306:PHE:HA	1.79	0.81
1:A:12:THR:HG22	1:A:13:ALA:H	1.45	0.81
1:A:269:MSE:O	1:A:269:MSE:CG	2.28	0.81
1:A:249:TRP:HB2	1:A:294:VAL:HG23	1.63	0.80
1:A:268:LYS:HG2	3:A:591:HOH:O	1.83	0.78
1:A:245:LYS:HE2	1:A:246:ARG:HG3	1.63	0.78
1:A:313:ASN:N	1:A:313:ASN:HD22	1.82	0.77
1:A:314:THR:O	1:A:314:THR:CG2	2.30	0.77
1:A:268:LYS:O	1:A:272:ASN:ND2	2.17	0.76
1:A:287:ASP:HB2	1:A:289:GLN:H	1.51	0.75
1:A:1:MSE:HE2	1:A:1:MSE:H1	1.50	0.75
1:A:285:LEU:HB3	3:A:453:HOH:O	1.87	0.74
1:A:52:MSE:HE2	1:A:58:LEU:CD1	2.10	0.73
1:A:62:HIS:HE2	1:A:98:LEU:HD23	1.53	0.73
1:A:5:PRO:HA	1:A:23:THR:HG21	1.71	0.73
1:A:194:ILE:HG21	1:A:291:VAL:HG12	1.71	0.73
1:A:53:ALA:HB3	1:A:56:GLN:HG3	1.69	0.73
1:A:87:ARG:HD2	1:A:200:VAL:CG1	2.19	0.72
1:A:88:ARG:NH2	1:A:113:ASP:OD1	2.24	0.71
1:A:212:GLN:HA	1:A:217:GLN:OE1	1.90	0.71
1:A:313:ASN:N	1:A:313:ASN:ND2	2.35	0.71
1:A:212:GLN:HB3	1:A:217:GLN:OE1	1.91	0.71
1:A:265:LEU:HD21	1:A:279:VAL:HG23	1.73	0.70
1:A:153:TRP:CH2	1:A:155:GLU:HB2	2.26	0.70
1:A:62:HIS:ND1	1:A:62:HIS:C	2.49	0.70
1:A:162:LEU:HD23	1:A:163:ILE:N	2.08	0.69
1:A:267:LEU:HD13	1:A:272:ASN:HB2	1.73	0.69
1:A:137:PRO:HB2	1:A:153:TRP:HB2	1.76	0.68
1:A:306:PHE:CE1	1:A:317:ILE:HD11	2.29	0.68
1:A:62:HIS:HE2	1:A:98:LEU:CD2	2.06	0.68
1:A:306:PHE:HE1	1:A:317:ILE:CD1	2.08	0.66
1:A:307:ARG:HD2	1:A:312:ALA:HA	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HD2	3:A:608:HOH:O	1.97	0.65
1:A:155:GLU:CG	1:A:156:HIS:CE1	2.80	0.65
1:A:205:ASN:N	1:A:205:ASN:ND2	2.37	0.65
1:A:249:TRP:CD1	1:A:296:MSE:HB2	2.32	0.65
1:A:49:VAL:HG12	1:A:49:VAL:O	1.97	0.64
1:A:234:MSE:HG2	1:A:237:ARG:HH22	1.56	0.63
1:A:260:GLU:O	1:A:279:VAL:CG1	2.46	0.63
1:A:62:HIS:NE2	1:A:98:LEU:CD2	2.62	0.63
1:A:49:VAL:O	1:A:49:VAL:CG1	2.47	0.63
1:A:162:LEU:HD23	1:A:162:LEU:C	2.24	0.63
1:A:212:GLN:NE2	1:A:235:VAL:HG13	2.14	0.63
1:A:92:GLU:HB3	1:A:93:PRO:HD3	1.80	0.63
1:A:23:THR:CG2	1:A:25:ASP:OD1	2.46	0.62
1:A:199:PRO:HB3	1:A:214:THR:HG23	1.82	0.62
1:A:87:ARG:HD2	1:A:200:VAL:HG13	1.80	0.61
1:A:158:ALA:O	1:A:159:GLU:CB	2.40	0.61
1:A:212:GLN:C	1:A:214:THR:H	2.10	0.60
1:A:86:GLU:CD	1:A:94:GLN:HE22	2.05	0.60
1:A:161:PHE:CD1	1:A:161:PHE:N	2.70	0.60
1:A:249:TRP:N	1:A:294:VAL:O	2.28	0.60
1:A:32:ILE:HD12	1:A:109:ILE:HG12	1.83	0.59
1:A:245:LYS:HG3	1:A:246:ARG:H	1.67	0.59
1:A:89:SER:O	1:A:203:ALA:HB2	2.02	0.59
1:A:275:ARG:O	1:A:275:ARG:HG2	2.02	0.59
1:A:6:PHE:H	1:A:23:THR:HG21	1.68	0.59
1:A:273:TRP:HA	1:A:273:TRP:CE3	2.37	0.59
1:A:301:GLU:C	1:A:303:ASP:N	2.61	0.59
1:A:86:GLU:CD	1:A:94:GLN:NE2	2.60	0.58
1:A:286:GLU:O	1:A:287:ASP:C	2.45	0.58
1:A:269:MSE:HB3	1:A:274:ARG:HH12	1.68	0.58
1:A:307:ARG:O	1:A:308:VAL:C	2.47	0.58
1:A:92:GLU:HB3	1:A:93:PRO:CD	2.33	0.58
1:A:260:GLU:O	1:A:279:VAL:HG11	2.02	0.58
1:A:52:MSE:SE	1:A:58:LEU:HD11	2.55	0.57
1:A:1:MSE:HE2	1:A:1:MSE:N	2.19	0.57
1:A:64:ASP:OD1	1:A:68:LYS:HB2	2.04	0.57
1:A:75:LEU:CD2	1:A:82:PHE:HB3	2.35	0.57
1:A:62:HIS:NE2	1:A:98:LEU:HD23	2.19	0.56
1:A:306:PHE:HE1	1:A:317:ILE:HD12	1.70	0.56
1:A:201:ILE:HG22	1:A:201:ILE:O	2.03	0.56
1:A:273:TRP:HA	1:A:273:TRP:HE3	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MSE:HE1	1:A:214:THR:HG21	1.87	0.56
1:A:267:LEU:HD21	1:A:304:SER:HB3	1.86	0.56
1:A:325:GLU:HA	1:A:325:GLU:OE1	2.05	0.56
1:A:10:GLN:HG2	1:A:286:GLU:HA	1.86	0.56
1:A:213:ALA:HB2	1:A:245:LYS:HZ3	1.71	0.56
1:A:247:ALA:O	1:A:295:VAL:HA	2.06	0.55
1:A:287:ASP:HB2	1:A:289:GLN:CG	2.30	0.55
1:A:298:ASN:OD1	1:A:298:ASN:N	2.26	0.55
1:A:301:GLU:C	1:A:303:ASP:H	2.07	0.55
1:A:70:TRP:CZ2	1:A:97:GLU:HG3	2.42	0.55
1:A:45:VAL:HG13	1:A:47:ALA:H	1.71	0.55
1:A:32:ILE:HA	1:A:108:THR:O	2.06	0.55
1:A:211:PRO:CB	1:A:222:ILE:HD11	2.37	0.54
1:A:62:HIS:CD2	1:A:98:LEU:HD21	2.41	0.54
1:A:14:SER:HB3	1:A:195:GLU:OE2	2.07	0.54
1:A:212:GLN:HE22	1:A:235:VAL:HG13	1.73	0.54
1:A:289:GLN:HB3	3:A:597:HOH:O	2.08	0.54
1:A:175:ASP:HA	3:A:556:HOH:O	2.07	0.54
1:A:15:ALA:HB2	3:A:421:HOH:O	2.06	0.54
1:A:227:GLY:O	1:A:228:CYS:HB2	2.07	0.54
1:A:245:LYS:HB2	1:A:246:ARG:HG3	1.90	0.54
1:A:265:LEU:HD21	1:A:279:VAL:CG2	2.38	0.54
1:A:253:GLY:O	1:A:290:VAL:HG23	2.08	0.54
1:A:251:LEU:CD2	1:A:317:ILE:HG13	2.38	0.53
1:A:229:TYR:CE1	1:A:232:GLN:HA	2.44	0.53
1:A:217:GLN:HG2	1:A:218:ALA:N	2.23	0.53
1:A:306:PHE:CE1	1:A:317:ILE:CD1	2.87	0.53
1:A:270:GLY:O	1:A:271:GLU:HG3	2.10	0.52
1:A:212:GLN:CB	1:A:217:GLN:OE1	2.57	0.52
1:A:64:ASP:CG	1:A:68:LYS:HB2	2.35	0.52
1:A:29:LEU:HD23	1:A:112:ASP:HB3	1.92	0.52
1:A:194:ILE:HG21	1:A:291:VAL:CG1	2.39	0.52
1:A:245:LYS:HE2	1:A:246:ARG:HD2	1.91	0.52
1:A:212:GLN:CA	1:A:217:GLN:OE1	2.59	0.51
1:A:251:LEU:HD22	1:A:317:ILE:HG13	1.93	0.51
1:A:1:MSE:N	1:A:1:MSE:CE	2.74	0.51
1:A:209:PHE:CE1	1:A:295:VAL:HG11	2.46	0.50
1:A:245:LYS:CG	1:A:246:ARG:H	2.24	0.50
1:A:120:VAL:HG21	1:A:129:LEU:HD21	1.93	0.50
1:A:153:TRP:CH2	1:A:155:GLU:CB	2.94	0.50
1:A:70:TRP:O	1:A:206:SER:CB	2.54	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HH21	1:A:309:ARG:CD	2.24	0.50
1:A:12:THR:HG22	1:A:13:ALA:N	2.22	0.50
1:A:162:LEU:C	1:A:162:LEU:CD2	2.85	0.50
1:A:89:SER:HA	3:A:589:HOH:O	2.11	0.49
1:A:269:MSE:HA	1:A:272:ASN:O	2.12	0.49
1:A:286:GLU:O	1:A:288:GLY:N	2.45	0.49
1:A:245:LYS:HE2	1:A:246:ARG:CG	2.36	0.49
1:A:274:ARG:HH21	1:A:307:ARG:HH22	1.59	0.49
1:A:211:PRO:HB3	1:A:222:ILE:HD11	1.94	0.49
1:A:280:LEU:CB	1:A:293:GLN:HG2	2.39	0.49
1:A:287:ASP:CB	1:A:289:GLN:CG	2.84	0.48
1:A:306:PHE:O	1:A:307:ARG:HB3	2.12	0.48
1:A:1:MSE:H1	1:A:1:MSE:CE	2.21	0.48
1:A:19:LEU:HD23	1:A:180:GLU:HG3	1.96	0.48
1:A:62:HIS:CD2	1:A:98:LEU:CD2	2.96	0.48
1:A:249:TRP:CD1	1:A:296:MSE:HE2	2.48	0.48
1:A:287:ASP:HB3	1:A:289:GLN:HG2	1.90	0.48
1:A:297:ASN:C	1:A:299:ASP:H	2.21	0.48
1:A:197:GLY:HA3	1:A:322:TYR:HE2	1.77	0.47
1:A:20:THR:HG22	1:A:22:MSE:HE2	1.96	0.47
1:A:143:VAL:HG22	1:A:152:LEU:HD22	1.96	0.47
1:A:260:GLU:O	1:A:279:VAL:HG12	2.14	0.47
1:A:297:ASN:C	1:A:299:ASP:N	2.72	0.47
1:A:233:GLU:O	1:A:237:ARG:HB2	2.15	0.47
1:A:49:VAL:CG1	1:A:82:PHE:CZ	2.99	0.46
1:A:250:LEU:HG	1:A:318:GLU:HB2	1.97	0.46
1:A:66:LYS:NZ	1:A:66:LYS:HB3	2.31	0.46
1:A:199:PRO:CB	1:A:214:THR:HG23	2.45	0.46
1:A:279:VAL:HA	1:A:294:VAL:HG12	1.98	0.46
1:A:211:PRO:HB2	1:A:222:ILE:HD11	1.97	0.46
1:A:1:MSE:C	1:A:3:PHE:N	2.74	0.46
1:A:275:ARG:HH21	1:A:309:ARG:HD3	1.81	0.46
1:A:190:LEU:O	1:A:194:ILE:HG13	2.15	0.46
1:A:312:ALA:C	1:A:313:ASN:ND2	2.73	0.45
1:A:7:PRO:HG2	3:A:487:HOH:O	2.16	0.45
1:A:226:LYS:CD	1:A:227:GLY:N	2.65	0.45
1:A:68:LYS:HG2	3:A:611:HOH:O	2.15	0.45
1:A:214:THR:O	1:A:214:THR:CG2	2.65	0.45
1:A:32:ILE:HD12	1:A:109:ILE:CG1	2.46	0.44
1:A:159:GLU:C	1:A:160:ARG:HG3	2.41	0.44
1:A:267:LEU:CD2	1:A:268:LYS:N	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:O	1:A:74:ARG:HA	2.17	0.44
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.76	0.44
1:A:52:MSE:HE3	1:A:52:MSE:HB2	1.69	0.44
1:A:304:SER:O	1:A:305:ILE:HD13	2.17	0.44
1:A:61:ALA:HB2	1:A:216:LEU:HD13	1.99	0.43
1:A:212:GLN:C	1:A:214:THR:N	2.75	0.43
1:A:240:PHE:C	1:A:242:GLY:N	2.71	0.43
1:A:99:LYS:HE3	1:A:99:LYS:HB2	1.53	0.43
1:A:10:GLN:HA	1:A:11:PRO:HD3	1.88	0.43
1:A:23:THR:CG2	1:A:23:THR:O	2.67	0.43
1:A:158:ALA:N	3:A:511:HOH:O	2.50	0.43
1:A:268:LYS:C	1:A:270:GLY:H	2.26	0.43
1:A:265:LEU:N	1:A:265:LEU:HD23	2.33	0.43
1:A:283:VAL:HG12	1:A:285:LEU:HD23	2.00	0.43
1:A:194:ILE:CG2	1:A:291:VAL:CG1	2.97	0.43
1:A:210:ILE:CG2	1:A:212:GLN:HG2	2.49	0.42
1:A:156:HIS:HA	1:A:157:PRO:C	2.44	0.42
1:A:162:LEU:HD12	2:A:400:SO4:O3	2.20	0.42
1:A:265:LEU:HD22	1:A:265:LEU:HA	1.75	0.42
1:A:212:GLN:HG2	1:A:212:GLN:H	1.21	0.42
1:A:245:LYS:HE2	1:A:246:ARG:CD	2.50	0.42
1:A:264:ASP:C	1:A:265:LEU:HD23	2.45	0.41
1:A:267:LEU:HB2	1:A:276:THR:OG1	2.20	0.41
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.76	0.41
1:A:313:ASN:HA	3:A:570:HOH:O	2.21	0.41
1:A:22:MSE:HB2	1:A:22:MSE:HE3	1.64	0.41
1:A:177:LEU:O	1:A:178:ARG:C	2.63	0.41
1:A:248:LEU:HD21	1:A:293:GLN:CD	2.46	0.41
1:A:279:VAL:HG12	1:A:279:VAL:O	2.20	0.41
1:A:266:GLU:OE2	1:A:309:ARG:CG	2.48	0.41
1:A:46:THR:HG21	1:A:61:ALA:HB3	2.02	0.41
1:A:265:LEU:CD2	1:A:279:VAL:HG23	2.47	0.41
1:A:64:ASP:OD2	1:A:68:LYS:HB2	2.20	0.41
1:A:202:ASP:O	1:A:203:ALA:C	2.64	0.40
1:A:210:ILE:O	1:A:213:ALA:N	2.49	0.40
1:A:93:PRO:O	1:A:94:GLN:C	2.64	0.40
1:A:23:THR:O	1:A:23:THR:HG22	2.20	0.40
1:A:203:ALA:O	1:A:204:ALA:C	2.64	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	324/328 (99%)	277 (86%)	35 (11%)	12 (4%)	2 9

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLU
1	A	245	LYS
1	A	273	TRP
1	A	287	ASP
1	A	123	PHE
1	A	314	THR
1	A	228	CYS
1	A	269	MSE
1	A	302	PRO
1	A	71	SER
1	A	158	ALA
1	A	308	VAL

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	265/256 (104%)	185 (70%)	80 (30%)	0 1

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	10	GLN
1	A	14	SER
1	A	17	LEU
1	A	22	MSE
1	A	23	THR
1	A	25	ASP
1	A	38	GLU
1	A	41	MSE
1	A	44	GLN
1	A	45	VAL
1	A	52	MSE
1	A	58	LEU
1	A	62	HIS
1	A	68	LYS
1	A	73	LEU
1	A	74	ARG
1	A	75	LEU
1	A	88	ARG
1	A	90	VAL
1	A	91	ARG
1	A	96	THR
1	A	98	LEU
1	A	99	LYS
1	A	105	SER
1	A	107	VAL
1	A	114	GLU
1	A	115	ARG
1	A	126	ARG
1	A	134	SER
1	A	155	GLU
1	A	159	GLU
1	A	160	ARG
1	A	167	GLU
1	A	178	ARG
1	A	180	GLU
1	A	201	ILE
1	A	205	ASN
1	A	208	GLN
1	A	210	ILE
1	A	212	GLN
1	A	214	THR
1	A	222	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	226	LYS
1	A	234	MSE
1	A	241	ARG
1	A	245	LYS
1	A	246	ARG
1	A	248	LEU
1	A	254	SER
1	A	256	SER
1	A	257	ARG
1	A	260	GLU
1	A	263	GLU
1	A	265	LEU
1	A	267	LEU
1	A	268	LYS
1	A	269	MSE
1	A	272	ASN
1	A	273	TRP
1	A	274	ARG
1	A	279	VAL
1	A	284	LYS
1	A	287	ASP
1	A	290	VAL
1	A	292	VAL
1	A	296	MSE
1	A	298	ASN
1	A	300	MSE
1	A	301	GLU
1	A	303	ASP
1	A	304	SER
1	A	307	ARG
1	A	309	ARG
1	A	311	ASP
1	A	313	ASN
1	A	314	THR
1	A	317	ILE
1	A	323	SER
1	A	324	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	124	GLN
1	A	205	ASN
1	A	313	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	SO4	A	400	-	4,4,4	0.27	0	6,6,6	0.43	0
2	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.33	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	315/328 (96%)	-0.48	11 (3%) 47 38	27, 57, 121, 145	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	TRP	3.6
1	A	263	GLU	3.1
1	A	243	ALA	3.1
1	A	270	GLY	3.0
1	A	286	GLU	2.6
1	A	299	ASP	2.4
1	A	314	THR	2.4
1	A	276	THR	2.3
1	A	2	ALA	2.1
1	A	311	ASP	2.1
1	A	312	ALA	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	401	5/5	0.89	0.12	49,52,55,57	5
2	SO4	A	400	5/5	0.92	0.10	25,34,48,53	5

6.5 Other polymers [i](#)

There are no such residues in this entry.