



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2017 – 06:05 PM EST

PDB ID : 5GMY
Title : Crystal structure of the Archaeoglobus fulgidus oligosaccharyltransferase (O29867_ARCFU) tethered with an acceptor peptide containing the NVT sequon via a disulfide bond
Authors : Matsumoto, S.; Kohda, D.
Deposited on : 2016-07-18
Resolution : 3.50 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

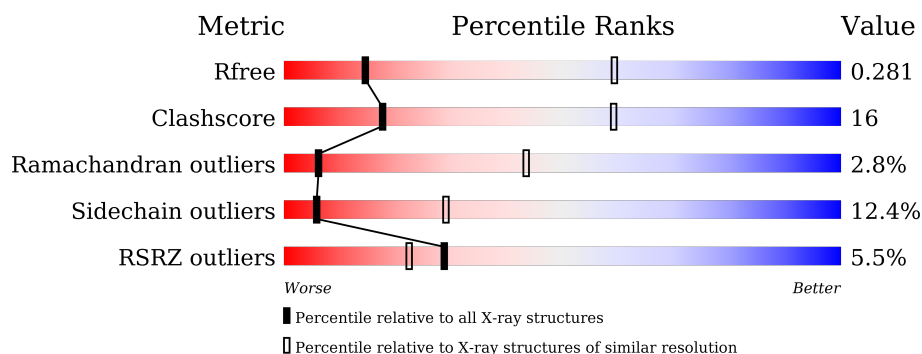
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	875	<div> <div>5%</div> <div>56%</div> <div>35%</div> <div>6%</div> <div>.</div> </div>
2	B	7	<div> <div>57%</div> <div>43%</div> <div>14%</div> <div>43%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	1200	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6887 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 Transmembrane oligosaccharyl transferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	848	Total	C	N	O	S	0	0	0
			6830	4540	1084	1189	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	617	CYS	GLY	engineered mutation	UNP O29867
A	869	GLU	-	expression tag	UNP O29867
A	870	LEU	-	expression tag	UNP O29867
A	871	ALA	-	expression tag	UNP O29867
A	872	LEU	-	expression tag	UNP O29867
A	873	VAL	-	expression tag	UNP O29867
A	874	PRO	-	expression tag	UNP O29867
A	875	ARG	-	expression tag	UNP O29867

- Molecule 2 is a protein called acceptor peptide, ARG-TYR-ASN-VAL-THR-ALA-CYS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	S	0	0	0
			56	34	11	10	1			

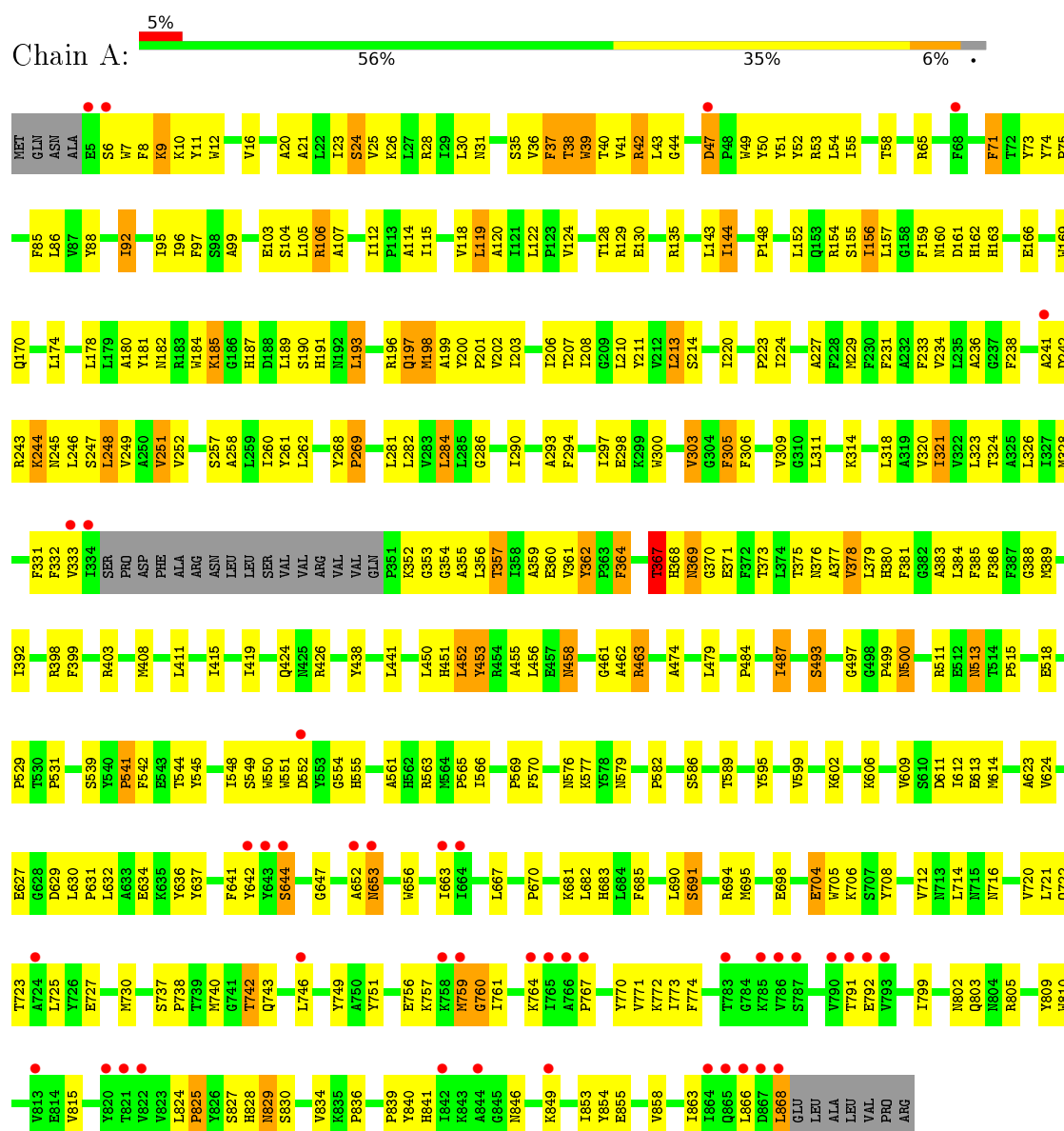
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

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: Transmembrane oligosaccharyl transferase, putative



- Molecule 2: acceptor peptide, ARG-TYR-ASN-VAL-THR-ALA-CYS



R11	Y12	M3	V14	T15	A16	G17

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.55Å 121.55Å 181.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.10 – 3.50 46.62 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (40.10-3.50) 98.9 (46.62-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.208 , 0.279 0.207 , 0.281	Depositor DCC
R_{free} test set	886 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	142.7	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6887	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: MG

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	0.34	0/7055	0.55	0/9627
2	B	0.33	0/56	0.71	0/75
All	All	0.34	0/7111	0.56	0/9702

There are no bond length outliers.

There are no bond angle outliers.

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	6830	0	6720	214	0
2	B	56	0	52	5	0
3	A	1	0	0	0	0
All	All	6887	0	6772	217	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 16.

All (217) 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:124:VAL:HG21	1:A:144:ILE:HG13	1.60	0.83
1:A:458:ASN:HA	1:A:462:ALA:H	1.44	0.82
1:A:156:ILE:HD11	1:A:493:SER:HB2	1.63	0.81
1:A:154:ARG:HH22	1:A:360:GLU:HG3	1.47	0.78
1:A:740:MET:HA	1:A:743:GLN:HE21	1.49	0.77
1:A:309:VAL:HG23	1:A:311:LEU:HB2	1.66	0.76
1:A:199:ALA:HA	1:A:202:VAL:HB	1.69	0.74
1:A:751:TYR:OH	1:A:760:GLY:O	2.07	0.71
1:A:511:ARG:HB2	1:A:561:ALA:HA	1.74	0.70
1:A:85:PHE:HB3	1:A:214:SER:HB3	1.72	0.70
1:A:451:HIS:O	1:A:453:TYR:N	2.25	0.68
1:A:551:TRP:HE3	1:A:569:PRO:HA	1.58	0.68
1:A:458:ASN:HD22	1:A:463:ARG:HA	1.59	0.68
1:A:243:ARG:O	1:A:247:SER:OG	2.08	0.67
1:A:162:HIS:H	1:A:162:HIS:HD1	1.41	0.66
1:A:37:PHE:HE2	1:A:157:LEU:HD21	1.61	0.66
1:A:545:TYR:HB2	1:A:606:LYS:HB2	1.78	0.65
1:A:28:ARG:NH1	1:A:152:LEU:HD12	2.12	0.65
1:A:849:LYS:HD2	1:A:866:LEU:HD21	1.79	0.63
1:A:637:TYR:HA	1:A:670:PRO:HA	1.81	0.63
1:A:378:VAL:HG13	1:A:386:PHE:HE2	1.63	0.62
1:A:698:GLU:HG3	1:A:772:LYS:HG2	1.82	0.62
1:A:829:ASN:OD1	1:A:855:GLU:N	2.31	0.61
1:A:318:LEU:HA	1:A:321:ILE:HB	1.82	0.61
1:A:180:ALA:HA	1:A:200:TYR:HB3	1.82	0.61
1:A:41:VAL:HG11	1:A:107:ALA:HA	1.83	0.61
1:A:551:TRP:CE3	1:A:569:PRO:HA	2.36	0.61
1:A:262:LEU:HD12	1:A:281:LEU:HD21	1.82	0.60
1:A:411:LEU:O	1:A:415:ILE:HG13	2.01	0.59
1:A:12:TRP:O	1:A:16:VAL:HG12	2.01	0.59
1:A:554:GLY:HA3	1:A:569:PRO:HD3	1.83	0.59
1:A:231:PHE:HA	1:A:234:VAL:HG22	1.85	0.59
1:A:356:LEU:HA	1:A:357:THR:HG22	1.85	0.59
1:A:40:THR:OG1	1:A:106:ARG:NH1	2.37	0.58
1:A:576:ASN:O	1:A:586:SER:HB3	2.04	0.58
1:A:24:SER:HB3	1:A:118:VAL:HG22	1.88	0.56
1:A:511:ARG:O	1:A:563:ARG:NH2	2.37	0.56
1:A:152:LEU:HD21	1:A:493:SER:HB3	1.87	0.56
1:A:354:GLY:HA2	1:A:355:ALA:HB3	1.88	0.56
1:A:297:ILE:HD11	1:A:323:LEU:HG	1.88	0.56
1:A:208:ILE:O	1:A:211:TYR:HB3	2.07	0.55
1:A:129:ARG:NH2	1:A:130:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:CE2	1:A:157:LEU:HD21	2.40	0.55
1:A:609:VAL:HG13	1:A:773:ILE:HG12	1.88	0.55
1:A:178:LEU:O	1:A:181:TYR:HB3	2.07	0.54
1:A:54:LEU:O	1:A:58:THR:OG1	2.16	0.54
1:A:114:ALA:HA	1:A:155:SER:O	2.07	0.54
1:A:377:ALA:HB1	1:A:385:PHE:CG	2.42	0.54
1:A:738:PRO:HB2	1:A:742:THR:HB	1.90	0.54
1:A:233:PHE:HB3	1:A:320:VAL:HG21	1.88	0.54
1:A:364:PHE:CE2	1:A:376:ASN:HB3	2.43	0.54
1:A:500:ASN:N	1:A:500:ASN:OD1	2.41	0.54
1:A:182:ASN:OD1	1:A:185:LYS:NZ	2.34	0.54
1:A:690:LEU:O	1:A:809:TYR:OH	2.18	0.54
1:A:206:ILE:O	1:A:210:LEU:HB2	2.08	0.54
1:A:213:LEU:HD11	1:A:261:TYR:HA	1.90	0.53
1:A:161:ASP:OD1	1:A:162:HIS:ND1	2.36	0.53
1:A:548:ILE:HB	1:A:566:ILE:HD13	1.91	0.53
1:A:698:GLU:O	1:A:803:GLN:NE2	2.38	0.53
1:A:378:VAL:HG13	1:A:386:PHE:CE2	2.43	0.53
1:A:683:HIS:CE1	1:A:772:LYS:HE3	2.44	0.53
1:A:802:ASN:N	1:A:802:ASN:OD1	2.36	0.53
1:A:577:LYS:NZ	1:A:636:TYR:OH	2.39	0.52
1:A:258:ALA:HB2	1:A:284:LEU:HB3	1.92	0.52
1:A:681:LYS:HA	1:A:685:PHE:HD2	1.75	0.52
1:A:120:ALA:O	1:A:124:VAL:HG23	2.09	0.52
1:A:360:GLU:HG2	1:A:426:ARG:HG3	1.91	0.52
2:B:11:ARG:NH2	2:B:12:TYR:HB3	2.25	0.52
1:A:759:MET:O	1:A:761:ILE:N	2.43	0.52
1:A:542:PHE:CZ	1:A:544:THR:HG22	2.45	0.52
1:A:828:HIS:NE2	1:A:839:PRO:HA	2.24	0.51
1:A:839:PRO:O	1:A:841:HIS:ND1	2.43	0.51
1:A:88:TYR:O	1:A:92:ILE:HG13	2.10	0.51
1:A:545:TYR:HB2	1:A:606:LYS:CB	2.40	0.51
1:A:187:HIS:HB3	1:A:191:HIS:ND1	2.26	0.51
1:A:582:PRO:HA	1:A:599:VAL:HG22	1.92	0.51
1:A:169:TRP:CH2	1:A:210:LEU:HD13	2.45	0.51
1:A:642:TYR:HE2	1:A:652:ALA:HB2	1.75	0.51
1:A:705:TRP:HA	1:A:708:TYR:HB2	1.92	0.50
1:A:849:LYS:NZ	1:A:868:LEU:HB3	2.26	0.50
1:A:257:SER:HA	1:A:260:ILE:HD12	1.91	0.50
1:A:399:PHE:CE2	1:A:408:MET:HB2	2.46	0.50
1:A:791:THR:HA	1:A:815:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:O	1:A:206:ILE:HG13	2.11	0.50
1:A:613:GLU:OE2	1:A:770:TYR:OH	2.22	0.50
1:A:233:PHE:CZ	1:A:243:ARG:HB3	2.47	0.50
1:A:642:TYR:CE2	1:A:652:ALA:HB2	2.47	0.50
1:A:7:TRP:CD1	1:A:8:PHE:HA	2.46	0.50
1:A:236:ALA:HA	1:A:243:ARG:NH2	2.27	0.50
1:A:629:ASP:HB3	1:A:632:LEU:HD13	1.94	0.50
1:A:306:PHE:O	1:A:311:LEU:HB3	2.12	0.49
1:A:359:ALA:HB2	2:B:16:ALA:HB2	1.94	0.49
1:A:694:ARG:HD3	1:A:825:PRO:O	2.12	0.49
1:A:154:ARG:HH21	2:B:12:TYR:HA	1.76	0.49
1:A:799:ILE:HA	1:A:836:PRO:HA	1.94	0.49
1:A:624:VAL:HG22	1:A:630:LEU:HA	1.95	0.49
1:A:49:TRP:O	1:A:52:TYR:HB3	2.14	0.48
1:A:40:THR:HG23	1:A:42:ARG:N	2.28	0.48
1:A:555:HIS:HE1	1:A:570:PHE:CD1	2.31	0.48
1:A:7:TRP:HA	1:A:9:LYS:N	2.27	0.48
1:A:242:ASP:OD2	1:A:245:ASN:ND2	2.46	0.48
1:A:611:ASP:HB3	1:A:771:VAL:HG22	1.95	0.48
1:A:21:ALA:O	1:A:25:VAL:HG23	2.14	0.48
1:A:383:ALA:HB2	1:A:484:PRO:HG2	1.94	0.48
1:A:369:ASN:N	1:A:369:ASN:OD1	2.46	0.48
1:A:756:GLU:O	1:A:757:LYS:NZ	2.47	0.47
1:A:529:PRO:O	1:A:531:PRO:HD3	2.13	0.47
1:A:582:PRO:HG3	1:A:602:LYS:HG2	1.95	0.47
1:A:682:LEU:HD22	1:A:774:PHE:CE2	2.49	0.47
1:A:364:PHE:HZ	1:A:380:HIS:HB2	1.79	0.47
1:A:47:ASP:N	1:A:47:ASP:OD1	2.48	0.47
1:A:220:ILE:HD12	1:A:223:PRO:HG3	1.97	0.47
1:A:555:HIS:CE1	1:A:569:PRO:HD2	2.49	0.47
1:A:286:GLY:O	1:A:290:ILE:HG13	2.14	0.47
1:A:853:ILE:HG21	1:A:858:VAL:HG23	1.96	0.47
1:A:623:ALA:O	1:A:627:GLU:HG2	2.14	0.47
1:A:644:SER:O	1:A:647:GLY:N	2.44	0.47
1:A:258:ALA:HA	1:A:284:LEU:HD23	1.96	0.46
1:A:71:PHE:O	1:A:565:PRO:HD2	2.16	0.46
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.83	0.46
1:A:7:TRP:NE1	1:A:11:TYR:HB2	2.31	0.46
1:A:178:LEU:O	1:A:182:ASN:ND2	2.48	0.46
1:A:392:ILE:HG12	1:A:438:TYR:CG	2.50	0.46
1:A:667:LEU:HD22	1:A:743:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:TRP:O	1:A:305:PHE:HB2	2.16	0.45
1:A:381:PHE:HB2	1:A:385:PHE:HB2	1.97	0.45
1:A:41:VAL:O	1:A:43:LEU:N	2.49	0.45
1:A:6:SER:O	1:A:9:LYS:HB2	2.16	0.45
1:A:203:ILE:HD12	1:A:206:ILE:HD12	1.97	0.45
1:A:49:TRP:HE1	1:A:499:PRO:HD3	1.82	0.45
1:A:86:LEU:HD12	1:A:162:HIS:HA	1.98	0.45
1:A:683:HIS:O	1:A:772:LYS:NZ	2.48	0.45
1:A:293:ALA:O	1:A:297:ILE:HG13	2.17	0.45
1:A:92:ILE:HG13	1:A:92:ILE:H	1.50	0.45
1:A:518:GLU:N	1:A:518:GLU:OE1	2.45	0.44
1:A:849:LYS:HZ1	1:A:868:LEU:HB3	1.80	0.44
1:A:9:LYS:HA	1:A:10:LYS:HA	1.70	0.44
2:B:12:TYR:CD1	2:B:14:VAL:HG22	2.52	0.44
1:A:721:LEU:HD11	1:A:749:TYR:CD2	2.52	0.44
1:A:555:HIS:CE1	1:A:570:PHE:HD1	2.36	0.44
1:A:51:TYR:CE1	1:A:86:LEU:HB3	2.52	0.44
1:A:355:ALA:O	1:A:356:LEU:HD13	2.17	0.44
1:A:364:PHE:CZ	1:A:376:ASN:HB3	2.52	0.44
1:A:224:ILE:O	1:A:227:ALA:HB3	2.17	0.44
1:A:555:HIS:HE1	1:A:570:PHE:HD1	1.65	0.44
1:A:695:MET:HE3	1:A:834:VAL:HG11	1.99	0.44
1:A:7:TRP:CD1	1:A:11:TYR:HB2	2.52	0.44
1:A:143:LEU:HD22	1:A:384:LEU:HD21	2.00	0.44
1:A:112:ILE:HG12	1:A:112:ILE:H	1.69	0.43
1:A:154:ARG:HG2	1:A:159:PHE:CE2	2.53	0.43
1:A:721:LEU:O	1:A:725:LEU:HG	2.18	0.43
2:B:11:ARG:CZ	2:B:12:TYR:HB3	2.48	0.43
1:A:184:TRP:CZ2	1:A:193:LEU:HG	2.53	0.43
1:A:352:LYS:HA	1:A:353:GLY:HA2	1.55	0.43
1:A:487:ILE:HD13	1:A:487:ILE:HA	1.58	0.43
1:A:555:HIS:CE1	1:A:570:PHE:CD1	3.06	0.43
1:A:38:THR:HB	1:A:39:TRP:H	1.51	0.43
1:A:799:ILE:HG12	1:A:836:PRO:HG3	2.00	0.43
1:A:74:TYR:HA	1:A:75:PRO:HA	1.70	0.43
1:A:827:SER:HB2	1:A:858:VAL:HG21	2.00	0.43
1:A:182:ASN:C	1:A:184:TRP:H	2.22	0.43
1:A:631:PRO:HA	1:A:634:GLU:HG2	2.00	0.43
1:A:189:LEU:HA	1:A:190:SER:HA	1.76	0.43
1:A:388:GLY:O	1:A:392:ILE:HG13	2.18	0.43
1:A:539:SER:O	1:A:541:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:LYS:HD2	1:A:706:LYS:HA	1.83	0.43
1:A:31:ASN:HB3	1:A:493:SER:O	2.20	0.42
1:A:324:THR:O	1:A:328:MET:HB2	2.19	0.42
1:A:103:GLU:HG2	1:A:106:ARG:NH1	2.35	0.42
1:A:99:ALA:HB1	1:A:104:SER:HB3	2.01	0.42
1:A:203:ILE:O	1:A:207:THR:HG23	2.19	0.42
1:A:691:SER:HA	1:A:825:PRO:HD3	2.01	0.42
1:A:196:ARG:C	1:A:198:MET:H	2.22	0.42
1:A:7:TRP:HE1	1:A:11:TYR:HB2	1.84	0.42
1:A:163:HIS:O	1:A:166:GLU:HB2	2.20	0.42
1:A:197:GLN:O	1:A:201:PRO:HD2	2.20	0.42
1:A:201:PRO:HB3	1:A:249:VAL:HB	2.00	0.42
1:A:361:VAL:HG12	1:A:424:GLN:HB3	2.02	0.42
1:A:549:SER:HB3	1:A:614:MET:HE1	2.01	0.42
1:A:248:LEU:O	1:A:252:VAL:HG23	2.20	0.42
1:A:115:ILE:O	1:A:119:LEU:HD22	2.19	0.42
1:A:849:LYS:HE2	1:A:849:LYS:HB2	1.91	0.41
1:A:248:LEU:O	1:A:251:VAL:HG13	2.20	0.41
1:A:367:THR:HB	1:A:368:HIS:H	1.48	0.41
1:A:453:TYR:C	1:A:455:ALA:H	2.22	0.41
1:A:698:GLU:OE1	1:A:805:ARG:NH2	2.50	0.41
1:A:714:LEU:HD12	1:A:767:PRO:HD2	2.02	0.41
1:A:824:LEU:HD13	1:A:840:TYR:CZ	2.55	0.41
1:A:92:ILE:HA	1:A:95:ILE:HG12	2.02	0.41
1:A:96:ILE:HG22	1:A:97:PHE:CD2	2.55	0.41
1:A:220:ILE:HD12	1:A:223:PRO:CG	2.51	0.41
1:A:290:ILE:O	1:A:293:ALA:HB3	2.20	0.41
1:A:550:TRP:H	1:A:614:MET:HE2	1.84	0.41
1:A:86:LEU:HD21	1:A:160:ASN:HD21	1.84	0.41
1:A:408:MET:O	1:A:411:LEU:HB2	2.20	0.41
1:A:50:TYR:HB2	1:A:555:HIS:CG	2.56	0.41
1:A:577:LYS:HD3	1:A:589:THR:OG1	2.21	0.41
1:A:314:LYS:H	1:A:314:LYS:HG2	1.71	0.41
1:A:399:PHE:O	1:A:403:ARG:N	2.46	0.41
1:A:44:GLY:HA2	1:A:497:GLY:O	2.20	0.41
1:A:20:ALA:HA	1:A:23:ILE:HD12	2.03	0.41
1:A:268:TYR:HA	1:A:269:PRO:HD2	1.77	0.41
1:A:721:LEU:HD11	1:A:749:TYR:CG	2.56	0.41
1:A:450:LEU:HB2	1:A:474:ALA:HB2	2.03	0.41
1:A:552:ASP:C	1:A:554:GLY:H	2.25	0.41
1:A:54:LEU:HD13	1:A:65:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ALA:O	1:A:105:LEU:HD23	2.21	0.41
1:A:247:SER:O	1:A:251:VAL:HG12	2.22	0.40
1:A:244:LYS:HG2	1:A:298:GLU:HG2	2.02	0.40
1:A:26:LYS:HA	1:A:30:LEU:HB2	2.02	0.40
1:A:143:LEU:HD13	1:A:384:LEU:HD22	2.04	0.40
1:A:563:ARG:HA	1:A:563:ARG:HD3	1.91	0.40
1:A:653:ASN:OD1	1:A:653:ASN:N	2.54	0.40
1:A:704:GLU:HG2	1:A:705:TRP:HD1	1.86	0.40
1:A:193:LEU:H	1:A:193:LEU:HD12	1.87	0.40
1:A:233:PHE:CZ	1:A:294:PHE:HB3	2.56	0.40
1:A:716:ASN:O	1:A:720:VAL:HG12	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	844/875 (96%)	710 (84%)	111 (13%)	23 (3%)	6	44
2	B	5/7 (71%)	2 (40%)	2 (40%)	1 (20%)	0	1
All	All	849/882 (96%)	712 (84%)	113 (13%)	24 (3%)	6	43

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	241	ALA
1	A	367	THR
1	A	452	LEU
1	A	213	LEU
1	A	515	PRO
1	A	759	MET

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Mol	Chain	Res	Type
1	A	760	GLY
2	B	12	TYR
1	A	36	VAL
1	A	37	PHE
1	A	303	VAL
1	A	369	ASN
1	A	513	ASN
1	A	541	PRO
1	A	579	ASN
1	A	362	TYR
1	A	9	LYS
1	A	148	PRO
1	A	269	PRO
1	A	825	PRO
1	A	333	VAL
1	A	370	GLY
1	A	461	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	704/728 (97%)	618 (88%)	86 (12%)	6	29
2	B	6/6 (100%)	4 (67%)	2 (33%)	0	2
All	All	710/734 (97%)	622 (88%)	88 (12%)	6	29

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	35	SER
1	A	38	THR
1	A	39	TRP
1	A	47	ASP
1	A	53	ARG

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Mol	Chain	Res	Type
1	A	55	ILE
1	A	71	PHE
1	A	73	TYR
1	A	92	ILE
1	A	106	ARG
1	A	119	LEU
1	A	122	LEU
1	A	128	THR
1	A	135	ARG
1	A	144	ILE
1	A	156	ILE
1	A	170	GLN
1	A	174	LEU
1	A	185	LYS
1	A	193	LEU
1	A	197	GLN
1	A	198	MET
1	A	229	MET
1	A	238	PHE
1	A	244	LYS
1	A	246	LEU
1	A	248	LEU
1	A	251	VAL
1	A	282	LEU
1	A	284	LEU
1	A	303	VAL
1	A	305	PHE
1	A	321	ILE
1	A	326	LEU
1	A	331	PHE
1	A	332	PHE
1	A	357	THR
1	A	362	TYR
1	A	364	PHE
1	A	367	THR
1	A	371	GLU
1	A	373	THR
1	A	375	THR
1	A	378	VAL
1	A	379	LEU
1	A	389	MET
1	A	398	ARG

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Mol	Chain	Res	Type
1	A	419	ILE
1	A	441	LEU
1	A	452	LEU
1	A	453	TYR
1	A	456	LEU
1	A	458	ASN
1	A	463	ARG
1	A	479	LEU
1	A	487	ILE
1	A	493	SER
1	A	500	ASN
1	A	513	ASN
1	A	595	TYR
1	A	612	ILE
1	A	641	PHE
1	A	644	SER
1	A	653	ASN
1	A	656	TRP
1	A	663	ILE
1	A	691	SER
1	A	704	GLU
1	A	712	VAL
1	A	722	GLN
1	A	723	THR
1	A	727	GLU
1	A	730	MET
1	A	737	SER
1	A	742	THR
1	A	746	LEU
1	A	764	LYS
1	A	792	GLU
1	A	810	TRP
1	A	829	ASN
1	A	830	SER
1	A	846	ASN
1	A	854	TYR
1	A	863	ILE
1	A	868	LEU
2	B	11	ARG
2	B	14	VAL

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

Mol	Chain	Res	Type
1	A	245	ASN
1	A	458	ASN
1	A	555	HIS
2	B	13	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	848/875 (96%)	0.14	43 (5%) 32 24	35, 85, 156, 209	0
2	B	7/7 (100%)	2.43	4 (57%) 0 0	91, 93, 115, 117	0
All	All	855/882 (96%)	0.16	47 (5%) 29 22	35, 86, 156, 209	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	792	GLU	6.6
2	B	17	CYS	5.7
1	A	765	ILE	4.9
1	A	793	VAL	4.5
1	A	866	LEU	4.3
1	A	664	ILE	3.6
1	A	758	LYS	3.5
1	A	844	ALA	3.4
1	A	786	VAL	3.3
1	A	764	LYS	3.2
1	A	334	ILE	3.2
1	A	868	LEU	3.1
1	A	822	VAL	3.1
1	A	766	ALA	3.1
1	A	785	LYS	3.1
1	A	643	TYR	3.0
1	A	842	ILE	3.0
1	A	865	GLN	2.9
1	A	813	VAL	2.9
1	A	864	ILE	2.9
1	A	6	SER	2.9
1	A	759	MET	2.8
1	A	5	GLU	2.8
1	A	849	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	333	VAL	2.7
1	A	644	SER	2.7
1	A	663	ILE	2.6
1	A	867	ASP	2.6
1	A	653	ASN	2.6
1	A	746	LEU	2.6
1	A	787	SER	2.5
1	A	790	VAL	2.5
1	A	724	ALA	2.4
1	A	652	ALA	2.4
1	A	68	PHE	2.4
1	A	767	PRO	2.3
1	A	642	TYR	2.3
1	A	820	TYR	2.3
1	A	783	THR	2.3
1	A	791	THR	2.3
2	B	13	ASN	2.2
1	A	821	THR	2.1
1	A	47	ASP	2.1
2	B	15	THR	2.1
2	B	16	ALA	2.1
1	A	241	ALA	2.0
1	A	552	ASP	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(\AA^2)	Q<0.9
3	MG	A	1200	1/1	0.86	0.89	4.53	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.