



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:04 PM UTC

PDB ID : 3FNB / pdb_00003fnb
Title : Crystal structure of acylaminoacyl peptidase SMU_737 from *Streptococcus mutans* UA159
Authors : Kim, Y.; Hatzos, C.; Cobb, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-12-23
Resolution : 2.12 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

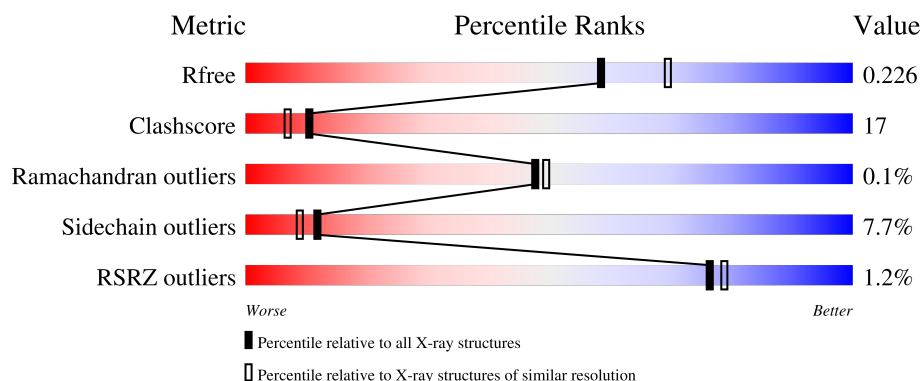
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	405	% 68% 21% • 8%
1	B	405	% 65% 22% • • 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6379 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 Acylaminoacyl peptidase SMU_737.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	Se	0	4	0
			3055	1960	510	570	5	10			
1	B	371	Total	C	N	O	S	Se	0	5	0
			3035	1946	505	569	5	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8DUZ1
A	-1	ASN	-	expression tag	UNP Q8DUZ1
A	0	ALA	-	expression tag	UNP Q8DUZ1
B	-2	SER	-	expression tag	UNP Q8DUZ1
B	-1	ASN	-	expression tag	UNP Q8DUZ1
B	0	ALA	-	expression tag	UNP Q8DUZ1

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	133	Total	O	0	0
			133	133		
6	B	118	Total	O	0	0
			118	118		

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.

Chain A:

68% 21% 8%

SER ASN ALA MSE LYS GLU ASN THR THR ILE L8 K9 R10 Q11 D12 Y13 C35 F36 N27 M27 M29 I35 L43 R61 H65 A66 D67 Y68 L69 V73 K77 K78 V79 G80 Y81 R82 D83 I85 S91 R97 L100 Q101 D104 P105 D107 F112 R115 R116 M117 M118 K119 M122 N127 S128 K129 E142 Y147 D153 R169 E170 D171 Y174 M175 S179 Y185 M186 Y187 L188 M189 V190 D191 L192 Q195 G196 K197 N198 L203 V207 T224 E225 K226 A230 G236 V243 E244 K245 I253 T256 P257 E283 V284 F285 R286 S287 F289 S290 K300 I311 N315 E319 I329 D330 F335 L336 V337 D342 S343 E344 L345 K346 R347 G348 S349 D354 N355 F356

Chain B:

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.83Å 56.47Å 99.90Å 90.00° 93.86° 90.00°	Depositor
Resolution (Å)	43.62 – 2.12 43.62 – 2.12	Depositor EDS
% Data completeness (in resolution range)	92.3 (43.62-2.12) 92.3 (43.62-2.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.173 , 0.225 (Not available) , 0.226	Depositor DCC
R_{free} test set	2060 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6379	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, EDO, BME, 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	0.72	0/3117	0.89	1/4190 (0.0%)
1	B	0.69	0/3097	0.90	9/4164 (0.2%)
All	All	0.71	0/6214	0.90	10/8354 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ILE	N-CA-C	-6.17	106.51	111.81
1	B	261	VAL	CB-CA-C	-6.07	103.85	112.22
1	B	149	ILE	CB-CA-C	5.67	118.07	110.42
1	B	337	VAL	N-CA-C	5.34	115.58	108.27
1	B	233	SER	CB-CA-C	-5.24	110.10	117.23
1	B	77	LYS	N-CA-C	-5.16	105.65	111.28
1	B	130	ILE	CA-C-N	5.16	126.28	119.84
1	B	130	ILE	C-N-CA	5.16	126.28	119.84
1	B	11	GLN	CA-C-N	-5.15	114.21	121.83
1	B	11	GLN	C-N-CA	-5.15	114.21	121.83

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	3055	0	2954	98	0
1	B	3035	0	2923	121	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	6	2	0
3	B	4	0	6	3	0
4	A	10	0	14	0	0
4	B	10	0	14	1	0
5	A	4	0	6	0	0
5	B	4	0	6	1	0
6	A	133	0	0	12	0
6	B	118	0	0	13	0
All	All	6379	0	5929	204	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 17.

All (204) 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:79:VAL:HB	1:B:81:TYR:CE2	1.87	1.09
1:B:221[B]:GLN:NE2	1:B:221[B]:GLN:HA	1.57	1.07
1:B:74:GLU:OE2	1:B:74:GLU:HA	1.40	1.07
1:B:221[B]:GLN:HA	1:B:221[B]:GLN:HE21	1.11	1.06
1:B:79:VAL:HG11	1:B:81:TYR:CZ	1.97	0.98
1:B:311:ILE:H	1:B:311:ILE:HD13	1.26	0.97
1:B:243:VAL:HG12	1:B:329:ILE:HD12	1.48	0.94
1:A:289:SER:OG	1:A:290:VAL:N	1.92	0.94
1:B:79:VAL:CB	1:B:81:TYR:CE2	2.53	0.91
1:A:392:GLU:HB3	1:B:81:TYR:CE1	2.07	0.90
1:A:300:LYS:HD2	6:A:480:HOH:O	1.74	0.86
1:B:79:VAL:CG1	1:B:81:TYR:CE2	2.59	0.85
1:A:13[B]:TYR:CD1	1:A:13[B]:TYR:O	2.30	0.85
1:A:392:GLU:OE1	1:B:81:TYR:CD1	2.32	0.82
1:B:311:ILE:H	1:B:311:ILE:CD1	1.92	0.82
1:A:392:GLU:CD	1:B:81:TYR:CD1	2.58	0.81
1:B:378:CYS:HG	3:B:403:BME:HS2	0.82	0.81
1:A:392:GLU:HB3	1:B:81:TYR:CD1	2.16	0.81
1:A:289:SER:OG	1:A:290:VAL:HG23	1.82	0.80
1:A:392:GLU:OE2	1:B:81:TYR:HB3	1.84	0.78
1:A:25[B]:CYS:SG	6:A:525:HOH:O	2.41	0.77
1:A:289:SER:HG	1:A:290:VAL:H	1.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLU:HB3	6:A:534:HOH:O	1.84	0.77
1:A:392:GLU:CD	1:B:81:TYR:HD1	1.93	0.76
1:A:81:TYR:HB3	1:B:392:GLU:OE1	1.87	0.75
1:A:82:ARG:HG2	1:A:127:ASN:O	1.87	0.74
1:B:311:ILE:HD13	1:B:311:ILE:N	2.01	0.74
1:A:192:LEU:H	1:A:195:GLN:HE21	1.34	0.74
1:B:79:VAL:HB	1:B:81:TYR:HE2	1.46	0.74
1:B:79:VAL:HG11	1:B:81:TYR:CE2	2.21	0.74
1:A:13[B]:TYR:O	1:A:13[B]:TYR:HD1	1.71	0.73
1:B:171:ASP:O	1:B:175:MSE:HG3	1.88	0.73
1:A:187:VAL:HG12	1:A:189:MSE:HE2	1.69	0.72
1:B:79:VAL:CG1	1:B:81:TYR:CZ	2.73	0.72
1:A:257:PRO:HG3	1:A:335:PHE:CD1	2.25	0.72
1:B:221[B]:GLN:HE21	1:B:221[B]:GLN:CA	1.91	0.72
1:A:175:MSE:HE1	3:A:403:BME:S2	2.31	0.71
1:A:9:LYS:HA	1:A:342:ASP:OD1	1.89	0.71
1:A:315:ASN:O	1:A:319:GLU:HG2	1.91	0.71
1:A:392:GLU:CG	1:B:81:TYR:HD1	2.03	0.71
1:B:311:ILE:CD1	1:B:311:ILE:N	2.53	0.71
1:A:8:LEU:HD12	6:A:522:HOH:O	1.91	0.70
1:B:35:ILE:HD11	1:B:383:PHE:HB2	1.71	0.70
1:B:79:VAL:O	1:B:79:VAL:HG12	1.90	0.70
1:B:77:LYS:O	1:B:79:VAL:N	2.26	0.69
1:A:13[A]:TYR:HE1	6:A:526:HOH:O	1.76	0.69
1:B:96:ILE:HD12	1:B:120:LEU:HD12	1.75	0.68
1:B:221[B]:GLN:NE2	1:B:221[B]:GLN:CA	2.41	0.67
1:A:82:ARG:CG	1:A:127:ASN:O	2.43	0.67
1:A:392:GLU:CD	1:B:81:TYR:HB3	2.21	0.66
1:B:131:PRO:HD2	1:B:149:ILE:CD1	2.26	0.66
1:A:104:ASP:O	1:A:107:ASP:HB2	1.95	0.66
1:B:131:PRO:HD2	1:B:149:ILE:HD11	1.77	0.66
1:A:346:MSE:HE1	1:A:367:LYS:NZ	2.11	0.65
1:B:180:GLY:HA2	1:B:391:PHE:CZ	2.31	0.65
1:A:392:GLU:HB3	1:B:81:TYR:HE1	1.57	0.65
1:A:207:VAL:HG12	6:A:467:HOH:O	1.96	0.65
1:B:237:TYR:CE1	1:B:261:VAL:HG22	2.32	0.65
1:A:73:VAL:HG13	1:A:85:ILE:HD12	1.79	0.65
1:B:96:ILE:HD12	1:B:120:LEU:CD1	2.27	0.64
1:B:79:VAL:HB	1:B:81:TYR:CD2	2.30	0.64
1:B:147:TYR:CE1	1:B:169:ARG:HG3	2.32	0.64
1:A:392:GLU:CB	1:B:81:TYR:CD1	2.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:OE2	1:B:377[A]:HIS:HD2	1.80	0.63
1:A:355:ASN:ND2	1:A:359:ARG:HH11	1.96	0.63
1:A:13[B]:TYR:HD1	1:A:13[B]:TYR:H	1.46	0.62
1:B:243:VAL:CG1	1:B:329:ILE:HG23	2.29	0.62
1:B:341:GLU:OE2	1:B:377[A]:HIS:CD2	2.53	0.62
1:B:171:ASP:HA	1:B:174:TYR:CE2	2.34	0.62
1:A:192:LEU:H	1:A:195:GLN:NE2	1.98	0.61
1:B:220:TYR:HA	6:B:511:HOH:O	2.00	0.61
1:A:378:CYS:SG	3:A:403:BME:S2	2.88	0.61
1:A:171:ASP:HA	1:A:174:TYR:CE2	2.36	0.60
1:B:378:CYS:SG	3:B:403:BME:S2	2.70	0.60
1:B:77:LYS:C	1:B:79:VAL:H	2.08	0.60
1:B:300[A]:LYS:HG3	1:B:304:GLN:HE21	1.66	0.60
1:B:192:LEU:H	1:B:195:GLN:HE21	1.49	0.60
1:B:149:ILE:HG12	1:B:181:TRP:CE3	2.37	0.59
1:A:263:GLU:HG3	1:A:267:ILE:HD12	1.84	0.59
1:B:79:VAL:HG11	1:B:81:TYR:OH	2.03	0.58
1:A:13[B]:TYR:CD1	1:A:13[B]:TYR:C	2.76	0.58
1:A:187:VAL:CG1	1:A:189:MSE:HE2	2.33	0.58
1:A:79:VAL:HG12	1:A:81:TYR:CE2	2.39	0.58
1:B:388:TYR:O	1:B:392:GLU:HG2	2.05	0.57
1:A:79:VAL:HG12	1:A:79:VAL:O	2.05	0.57
1:B:244:GLU:HA	1:B:329:ILE:HD13	1.87	0.57
1:A:115:ARG:O	1:A:119:LYS:HG3	2.06	0.56
1:A:175:MSE:CE	1:A:378:CYS:HB3	2.36	0.56
1:B:76:VAL:HG11	1:B:84:LEU:HD23	1.88	0.56
1:A:257:PRO:HG3	1:A:335:PHE:CG	2.41	0.55
1:B:60:LYS:O	1:B:64:GLU:HG3	2.05	0.55
1:B:74:GLU:OE2	1:B:74:GLU:CA	2.30	0.55
1:A:346:MSE:HG2	6:A:529:HOH:O	2.07	0.55
1:B:169:ARG:HD3	6:B:444:HOH:O	2.07	0.54
1:B:210:ARG:HG3	1:B:245:LYS:HE2	1.89	0.54
1:B:338:GLY:O	1:B:341:GLU:HB2	2.08	0.54
1:B:136:GLU:HB3	1:B:143:LEU:HB3	1.90	0.53
1:A:374:ALA:HB2	1:A:382:ASN:HB3	1.90	0.53
1:A:268:SER:HB3	1:A:269:PHE:CE2	2.44	0.53
1:B:237:TYR:CZ	1:B:261:VAL:HG22	2.44	0.52
1:A:118:GLU:OE2	1:A:197:LYS:HE3	2.10	0.52
1:A:355:ASN:HD21	1:A:359:ARG:HH11	1.57	0.52
1:A:392:GLU:CB	1:B:81:TYR:HD1	2.21	0.52
1:B:335:PHE:HB2	1:B:365:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLU:CG	1:B:81:TYR:CD1	2.91	0.52
1:B:79:VAL:CG1	1:B:79:VAL:O	2.58	0.51
1:B:11:GLN:N	1:B:340:GLY:HA3	2.24	0.51
1:B:396:HIS:O	1:B:400:LYS:HB2	2.10	0.51
1:A:13[B]:TYR:CD1	1:A:13[B]:TYR:N	2.66	0.51
1:A:169:ARG:HG3	1:A:191:ASP:OD2	2.10	0.51
1:A:185:TYR:OH	1:A:395:ASN:ND2	2.44	0.51
1:B:35:ILE:HD11	1:B:383:PHE:CB	2.40	0.51
1:B:132:LEU:HD23	1:B:133:LYS:N	2.26	0.51
1:B:35:ILE:HD12	1:B:35:ILE:N	2.26	0.51
1:B:132:LEU:HD23	1:B:132:LEU:C	2.36	0.51
1:A:81:TYR:CD2	1:B:392:GLU:HB3	2.46	0.51
1:B:36:ILE:H	1:B:36:ILE:HD12	1.76	0.51
1:B:250:LYS:HE2	6:B:446:HOH:O	2.10	0.50
1:A:81:TYR:CB	1:B:392:GLU:OE1	2.59	0.50
1:A:226:LYS:NZ	1:A:398:PHE:O	2.45	0.50
1:A:81:TYR:CE2	1:B:392:GLU:HB3	2.46	0.50
1:A:169:ARG:HD2	6:A:409:HOH:O	2.12	0.50
1:B:337:VAL:CG1	1:B:365:LEU:HD11	2.42	0.49
1:B:96:ILE:CD1	1:B:120:LEU:CD1	2.90	0.49
1:A:67:ASP:OD1	1:A:116:ARG:NH2	2.46	0.49
1:A:175:MSE:HE2	1:A:378:CYS:HB3	1.95	0.49
1:A:25[B]:CYS:O	1:A:29:MSE:HG2	2.13	0.48
1:B:374:ALA:HB2	1:B:382:ASN:HB3	1.94	0.48
1:B:76:VAL:O	1:B:77:LYS:C	2.53	0.48
1:A:11:GLN:NE2	1:A:27:ASN:HD22	2.12	0.48
1:B:79:VAL:CB	1:B:81:TYR:HE2	2.11	0.47
1:B:293:VAL:HG23	6:B:514:HOH:O	2.13	0.47
1:A:346:MSE:HE1	1:A:367:LYS:HZ3	1.77	0.47
1:B:72:GLU:O	1:B:76:VAL:HG23	2.14	0.47
1:B:118:GLU:OE2	1:B:197:LYS:HE3	2.14	0.46
1:B:46:ILE:HD11	1:B:65:HIS:CG	2.50	0.46
1:B:212:ALA:O	1:B:215:ALA:HB3	2.16	0.46
1:A:79:VAL:CG1	1:A:81:TYR:CE2	2.99	0.46
1:A:65:HIS:HE1	1:B:371[B]:GLU:O	1.99	0.46
1:B:111:MSE:HG2	6:B:480:HOH:O	2.16	0.45
1:A:25[A]:CYS:SG	1:A:101:GLN:HG2	2.56	0.45
1:A:257:PRO:HD2	1:A:349:SER:OG	2.16	0.45
1:A:197:LYS:HG2	6:A:436:HOH:O	2.17	0.45
1:B:77:LYS:C	1:B:79:VAL:N	2.66	0.45
1:A:77:LYS:C	1:A:79:VAL:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:SER:HB3	1:A:391:PHE:CE2	2.51	0.45
1:B:300[A]:LYS:HG3	1:B:304:GLN:NE2	2.32	0.45
1:A:169:ARG:HG3	1:A:169:ARG:H	1.56	0.45
1:B:341:GLU:HG3	6:B:504:HOH:O	2.17	0.45
1:A:85:ILE:HD13	1:A:85:ILE:HA	1.85	0.44
1:B:33:GLY:HA3	6:B:512:HOH:O	2.17	0.44
1:B:210:ARG:HD2	1:B:210:ARG:C	2.42	0.44
1:B:326:TYR:HA	1:B:329:ILE:HG12	1.99	0.44
4:B:404:PGE:H5	5:B:405:EDO:O1	2.18	0.44
1:B:94:PHE:HA	1:B:97:ARG:HB3	1.99	0.44
1:B:110:PHE:HB3	6:B:479:HOH:O	2.17	0.44
1:A:69:LEU:HD13	1:A:91:SER:HB2	2.00	0.44
1:B:25[B]:CYS:O	1:B:29:MSE:HG2	2.18	0.44
1:B:11:GLN:HB3	6:B:459:HOH:O	2.18	0.43
1:B:322:GLN:HE21	1:B:322:GLN:HB3	1.62	0.43
1:B:36:ILE:HD12	1:B:36:ILE:N	2.33	0.43
1:B:377[B]:HIS:CE1	6:B:504:HOH:O	2.70	0.43
1:B:137:VAL:HA	1:B:138:PRO:HD3	1.85	0.43
1:B:230:ALA:HA	1:B:253:ILE:O	2.17	0.43
1:A:330:ASP:C	6:A:512:HOH:O	2.61	0.43
1:B:319:GLU:HB3	1:B:320:GLN:HG3	2.00	0.43
1:A:356:PHE:HB3	1:A:361:ILE:HB	2.01	0.43
1:A:61:ARG:HA	1:A:61:ARG:HD3	1.91	0.43
1:B:87:HIS:NE2	6:B:506:HOH:O	2.37	0.43
1:A:147:TYR:CE2	1:A:169:ARG:HB2	2.54	0.42
1:A:230:ALA:HA	1:A:253:ILE:O	2.19	0.42
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.20	0.42
1:A:263:GLU:HG3	1:A:267:ILE:CD1	2.47	0.42
1:A:236:GLY:HA3	1:A:256:THR:O	2.19	0.42
1:A:354:ASP:HB3	6:A:516:HOH:O	2.20	0.42
1:B:149:ILE:HD11	1:B:181:TRP:CE2	2.55	0.42
1:A:129:LYS:HD3	6:A:490:HOH:O	2.19	0.42
1:B:346:MSE:HE1	1:B:367:LYS:HG2	2.01	0.42
1:A:192:LEU:N	1:A:195:GLN:HE21	2.09	0.42
1:B:82:ARG:HB2	6:B:478:HOH:O	2.19	0.42
1:A:311:ILE:HD13	1:A:311:ILE:HA	1.80	0.42
1:B:36:ILE:HD12	1:B:36:ILE:O	2.20	0.42
1:B:132:LEU:HD21	1:B:147:TYR:CD2	2.54	0.42
1:A:226:LYS:HG3	1:A:398:PHE:CD1	2.55	0.41
1:B:110:PHE:CE1	1:B:300[A]:LYS:HE2	2.56	0.41
3:B:403:BME:H11	6:B:410:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.94	0.41
1:B:315:ASN:O	1:B:319:GLU:HB2	2.20	0.41
1:A:97:ARG:HD3	1:A:97:ARG:C	2.45	0.41
1:A:243:VAL:HG13	1:A:329:ILE:HG23	2.03	0.41
1:B:236:GLY:HA3	1:B:256:THR:O	2.20	0.41
1:B:13:TYR:CD2	1:B:13:TYR:C	2.99	0.41
1:B:198:ASN:N	1:B:199:PRO:CD	2.84	0.41
1:A:265:PHE:O	1:A:266:ARG:C	2.64	0.41
1:B:356:PHE:HB3	1:B:361:ILE:HB	2.03	0.41
1:B:310:PHE:N	1:B:311:ILE:HD13	2.36	0.41
1:A:104:ASP:HA	1:A:105:PRO:HD3	1.87	0.40
1:A:79:VAL:O	1:A:79:VAL:CG1	2.69	0.40
1:B:46:ILE:HD11	1:B:65:HIS:CD2	2.56	0.40
1:A:84:LEU:HD12	1:A:84:LEU:O	2.21	0.40
1:B:155:ALA:HA	1:B:223:PRO:HB3	2.04	0.40
1:A:9:LYS:NZ	1:A:342:ASP:OD2	2.46	0.40
1:A:195:GLN:O	1:A:198:ASN:HB2	2.22	0.40
1:B:11:GLN:HE21	1:B:11:GLN:HB2	1.66	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	374/405 (92%)	359 (96%)	15 (4%)	0	100	100
1	B	372/405 (92%)	352 (95%)	19 (5%)	1 (0%)	36	36
All	All	746/810 (92%)	711 (95%)	34 (5%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	78	LYS

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	312/337 (93%)	287 (92%)	25 (8%)	11	8
1	B	316/337 (94%)	293 (93%)	23 (7%)	13	10
All	All	628/674 (93%)	580 (92%)	48 (8%)	12	9

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	43	LEU
1	A	100	LEU
1	A	107	ASP
1	A	112	GLU
1	A	122	MSE
1	A	129	LYS
1	A	153	ASP
1	A	169	ARG
1	A	179	SER
1	A	203	LEU
1	A	224	THR
1	A	226	LYS
1	A	243	VAL
1	A	244	GLU
1	A	245	LYS
1	A	270	SER
1	A	289	SER
1	A	290	VAL
1	A	300	LYS
1	A	311	ILE
1	A	319	GLU
1	A	337	VAL

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Mol	Chain	Res	Type
1	A	347	ARG
1	A	384	ARG
1	B	11	GLN
1	B	20	LYS
1	B	36	ILE
1	B	60	LYS
1	B	74	GLU
1	B	75	ARG
1	B	97	ARG
1	B	142	GLU
1	B	149	ILE
1	B	152	GLU
1	B	169	ARG
1	B	189	MSE
1	B	197	LYS
1	B	210	ARG
1	B	224	THR
1	B	243	VAL
1	B	261	VAL
1	B	311	ILE
1	B	319	GLU
1	B	322	GLN
1	B	337	VAL
1	B	366	ARG
1	B	386	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	195	GLN
1	A	221	GLN
1	A	297	ASN
1	A	307	GLN
1	A	320	GLN
1	A	355	ASN
1	A	379	GLN
1	A	395	ASN
1	B	18	ASN
1	B	63	ASN
1	B	195	GLN
1	B	304	GLN

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Mol	Chain	Res	Type
1	B	320	GLN
1	B	322	GLN
1	B	389	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	EDO	A	405	-	3,3,3	0.35	0	2,2,2	0.24	0
3	BME	B	403	-	3,3,3	0.40	0	2,2,2	1.33	0
4	PGE	B	404	-	9,9,9	0.40	0	8,8,8	0.44	0
4	PGE	A	404	-	9,9,9	0.68	0	8,8,8	1.36	1 (12%)
5	EDO	B	405	-	3,3,3	0.42	0	2,2,2	0.38	0
3	BME	A	403	-	3,3,3	0.42	0	2,2,2	1.35	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
5	EDO	A	405	-	-	1/1/1/1	-
3	BME	B	403	-	-	1/1/1/1	-
4	PGE	B	404	-	-	4/7/7/7	-
4	PGE	A	404	-	-	5/7/7/7	-
5	EDO	B	405	-	-	1/1/1/1	-
3	BME	A	403	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	PGE	C3-O2-C2	2.05	122.25	113.26

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	BME	O1-C1-C2-S2
4	B	404	PGE	O2-C3-C4-O3
4	A	404	PGE	O1-C1-C2-O2
5	A	405	EDO	O1-C1-C2-O2
4	A	404	PGE	O3-C5-C6-O4
5	B	405	EDO	O1-C1-C2-O2
4	A	404	PGE	O2-C3-C4-O3
4	B	404	PGE	O3-C5-C6-O4
4	B	404	PGE	C6-C5-O3-C4
4	A	404	PGE	C6-C5-O3-C4
4	A	404	PGE	C3-C4-O3-C5
4	B	404	PGE	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	BME	3	0
4	B	404	PGE	1	0
5	B	405	EDO	1	0
3	A	403	BME	2	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 [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	364/405 (89%)	-0.26	3 (0%) 82 85	16, 44, 82, 122	4 (1%)
1	B	361/405 (89%)	-0.06	6 (1%) 69 71	15, 51, 89, 140	5 (1%)
All	All	725/810 (89%)	-0.16	9 (1%) 76 79	15, 46, 88, 140	9 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	LEU	5.5
1	B	81	TYR	3.7
1	B	290	VAL	3.6
1	A	13[A]	TYR	3.5
1	B	13	TYR	3.4
1	B	80	GLY	2.7
1	A	81	TYR	2.5
1	B	82	ARG	2.1
1	B	78	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	405	4/4	0.84	0.16	76,77,78,81	0
2	MG	B	501	1/1	0.87	0.11	68,68,68,68	0
4	PGE	A	404	10/10	0.88	0.13	69,73,75,75	0
3	BME	B	403	4/4	0.88	0.14	70,71,74,77	0
4	PGE	B	404	10/10	0.90	0.11	73,78,82,83	0
5	EDO	A	405	4/4	0.90	0.12	45,53,63,65	0
2	MG	A	501	1/1	0.90	0.09	52,52,52,52	0
3	BME	A	403	4/4	0.91	0.13	69,72,74,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.