



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:13 AM UTC

PDB ID : 1FNO / pdb_00001fno
Title : PEPTIDASE T (TRIPPEPTIDASE)
Authors : Hakansson, K.; Miller, C.G.
Deposited on : 2000-08-22
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

<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

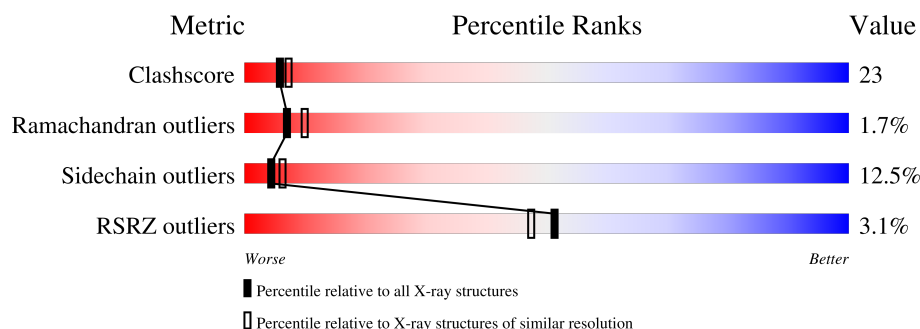
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	417	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3260 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 PEPTIDASE T.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	408	3118	1974	535	591	3	15	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P26311
A	45	MSE	MET	modified residue	UNP P26311
A	59	MSE	MET	modified residue	UNP P26311
A	116	MSE	MET	modified residue	UNP P26311
A	149	MSE	MET	modified residue	UNP P26311
A	231	MSE	MET	modified residue	UNP P26311
A	266	MSE	MET	modified residue	UNP P26311
A	275	MSE	MET	modified residue	UNP P26311
A	294	MSE	MET	modified residue	UNP P26311
A	295	MSE	MET	modified residue	UNP P26311
A	322	MSE	MET	modified residue	UNP P26311
A	340	MSE	MET	modified residue	UNP P26311
A	349	MSE	MET	modified residue	UNP P26311
A	364	MSE	MET	modified residue	UNP P26311
A	390	MSE	MET	modified residue	UNP P26311
A	410	LEU	-	expression tag	UNP P26311
A	411	GLU	-	expression tag	UNP P26311
A	412	HIS	-	expression tag	UNP P26311
A	413	HIS	-	expression tag	UNP P26311
A	414	HIS	-	expression tag	UNP P26311
A	415	HIS	-	expression tag	UNP P26311
A	416	HIS	-	expression tag	UNP P26311
A	417	HIS	-	expression tag	UNP P26311

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

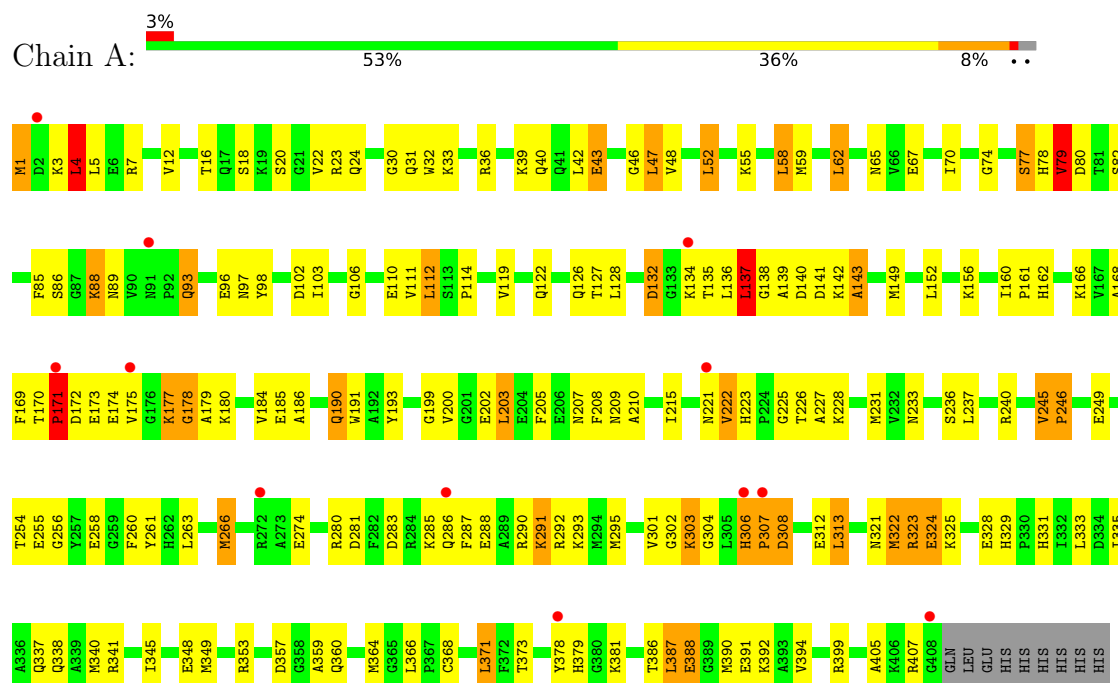
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		

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: PEPTIDASE T



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.37Å 46.04Å 96.59Å 90.00° 116.11° 90.00°	Depositor
Resolution (Å)	500.00 – 2.40 86.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (500.00-2.40) 95.4 (86.73-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.39 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.261 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 72.7	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	0.94	EDS
Total number of atoms	3260	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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, ZN

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	0.67	0/3165	1.17	27/4257 (0.6%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ASN	N-CA-C	-8.89	94.75	109.24
1	A	82	SER	N-CA-C	8.80	119.72	109.60
1	A	378	TYR	N-CA-C	8.58	125.53	111.37
1	A	306	HIS	CA-C-N	8.45	130.41	119.84
1	A	306	HIS	C-N-CA	8.45	130.41	119.84
1	A	308	ASP	N-CA-C	-8.00	102.79	114.39
1	A	379	HIS	N-CA-C	7.82	122.54	112.92
1	A	171	PRO	N-CA-C	7.65	128.22	112.47
1	A	111	VAL	N-CA-C	7.15	117.79	108.35
1	A	170	THR	CA-C-N	6.68	128.19	119.84
1	A	170	THR	C-N-CA	6.68	128.19	119.84
1	A	178	GLY	N-CA-C	6.36	120.59	112.83
1	A	287	PHE	N-CA-C	-6.07	104.23	111.69
1	A	112	LEU	N-CA-C	-6.00	98.95	108.73
1	A	261	TYR	N-CA-C	-5.84	99.87	109.40
1	A	291	LYS	N-CA-C	-5.84	104.55	111.03
1	A	143	ALA	N-CA-C	-5.82	105.02	111.36
1	A	137	LEU	N-CA-C	-5.81	105.20	112.93
1	A	22	VAL	N-CA-C	-5.74	100.02	108.85
1	A	132	ASP	N-CA-C	-5.67	106.13	113.16
1	A	199	GLY	N-CA-C	5.45	118.33	112.33
1	A	245	VAL	CA-C-N	5.35	126.53	119.84
1	A	245	VAL	C-N-CA	5.35	126.53	119.84
1	A	139	ALA	N-CA-C	-5.14	105.11	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	CYS	N-CA-C	5.14	117.75	108.55
1	A	79	VAL	N-CA-C	5.02	120.64	113.16
1	A	4	LEU	N-CA-C	-5.02	105.50	110.97

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	3118	0	3100	143	0
2	A	2	0	0	0	0
3	A	10	0	0	1	0
4	A	130	0	0	2	0
All	All	3260	0	3100	143	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 23.

All (143) 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:292:ARG:HA	1:A:295:MSE:HE3	1.42	0.98
1:A:93:GLN:NE2	1:A:106:GLY:H	1.67	0.93
1:A:93:GLN:HE22	1:A:106:GLY:H	0.90	0.87
1:A:93:GLN:HE22	1:A:106:GLY:N	1.74	0.84
1:A:258:GLU:O	1:A:353:ARG:NH2	2.15	0.79
1:A:227:ALA:HB1	1:A:231:MSE:HB2	1.64	0.79
1:A:175:VAL:HG12	1:A:175:VAL:O	1.83	0.78
1:A:193:TYR:HB3	1:A:371:LEU:HD23	1.66	0.78
1:A:210:ALA:HB1	1:A:280:ARG:NH2	2.00	0.77
1:A:306:HIS:O	1:A:308:ASP:N	2.15	0.77
1:A:16:THR:HG22	1:A:80:ASP:HA	1.69	0.74
1:A:255:GLU:O	1:A:258:GLU:HG2	1.86	0.74
1:A:65:ASN:ND2	1:A:160:ILE:O	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLU:HG2	1:A:325:LYS:N	2.04	0.72
1:A:42:LEU:HG	1:A:149:MSE:HE1	1.74	0.70
1:A:16:THR:HG22	1:A:16:THR:O	1.92	0.69
1:A:85:PHE:CE1	1:A:135:THR:HA	2.27	0.69
1:A:345:ILE:HD11	1:A:392:LYS:HD3	1.77	0.67
1:A:85:PHE:HE1	1:A:135:THR:HA	1.60	0.67
1:A:227:ALA:HB1	1:A:231:MSE:CB	2.25	0.66
1:A:16:THR:HG23	1:A:31:GLN:HA	1.77	0.66
1:A:231:MSE:CE	1:A:233:ASN:HB2	2.27	0.65
1:A:236:SER:O	1:A:240:ARG:HG3	1.97	0.65
1:A:16:THR:HG21	1:A:79:VAL:O	1.96	0.64
1:A:46:GLY:HA3	1:A:156:LYS:NZ	2.12	0.64
1:A:59:MSE:HE1	1:A:186:ALA:CB	2.29	0.63
1:A:203:LEU:HD12	1:A:340:MSE:HE1	1.80	0.63
1:A:190:GLN:HG2	1:A:191:TRP:HE3	1.65	0.62
1:A:143:ALA:HB3	1:A:373:THR:CG2	2.30	0.61
1:A:86:SER:O	1:A:135:THR:HB	2.00	0.61
1:A:329:HIS:HB3	1:A:331:HIS:CE1	2.35	0.61
1:A:193:TYR:CB	1:A:371:LEU:HD23	2.29	0.61
1:A:102:ASP:OD2	1:A:114:PRO:HD2	2.01	0.60
1:A:208:PHE:CD1	1:A:280:ARG:HB3	2.37	0.60
1:A:322:MSE:HG2	1:A:359:ALA:HA	1.83	0.59
1:A:32:TRP:O	1:A:36:ARG:HG3	2.02	0.58
1:A:23:ARG:HG2	1:A:23:ARG:HH11	1.68	0.58
1:A:62:LEU:HD13	1:A:162:HIS:CE1	2.39	0.58
1:A:175:VAL:O	1:A:175:VAL:CG1	2.52	0.58
1:A:128:LEU:CD2	1:A:386:THR:HG22	2.34	0.58
1:A:205:PHE:CE1	1:A:349:MSE:HE2	2.40	0.57
1:A:173:GLU:HG2	1:A:357:ASP:OD1	2.06	0.56
1:A:98:TYR:CE2	1:A:103:ILE:HD11	2.41	0.56
1:A:110:GLU:HA	1:A:110:GLU:OE1	2.07	0.55
1:A:215:ILE:HG12	1:A:313:LEU:HD22	1.87	0.55
1:A:335:ILE:HD11	1:A:407:ARG:HD3	1.89	0.55
1:A:338:GLN:NE2	1:A:341:ARG:HH21	2.04	0.54
1:A:207:ASN:OD1	1:A:322:MSE:HG3	2.06	0.54
1:A:185:GLU:HA	1:A:185:GLU:OE2	2.07	0.54
1:A:103:ILE:HB	1:A:112:LEU:HB3	1.88	0.54
1:A:65:ASN:HD22	1:A:161:PRO:HA	1.73	0.54
1:A:128:LEU:HD22	1:A:386:THR:HG22	1.90	0.54
1:A:103:ILE:HD13	1:A:112:LEU:HD12	1.90	0.54
1:A:16:THR:CG2	1:A:31:GLN:HG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLY:HA3	1:A:357:ASP:OD1	2.09	0.53
1:A:135:THR:O	1:A:381:LYS:HA	2.09	0.53
1:A:179:ALA:HB1	1:A:364:MSE:HE1	1.91	0.53
1:A:292:ARG:CA	1:A:295:MSE:HE3	2.30	0.53
1:A:303:LYS:CG	1:A:304:GLY:N	2.71	0.53
1:A:1:MSE:HG3	1:A:394:VAL:HG11	1.92	0.52
1:A:260:PHE:CZ	1:A:280:ARG:HG3	2.45	0.52
1:A:210:ALA:HB1	1:A:280:ARG:CZ	2.40	0.52
1:A:143:ALA:HB3	1:A:373:THR:HG21	1.91	0.51
1:A:172:ASP:HB2	1:A:177:LYS:HB2	1.92	0.51
1:A:222:VAL:HG12	1:A:223:HIS:O	2.11	0.51
1:A:360:GLN:C	1:A:364:MSE:HE3	2.36	0.51
1:A:203:LEU:HD12	1:A:340:MSE:CE	2.41	0.51
1:A:32:TRP:HZ3	1:A:52:LEU:HD13	1.76	0.51
1:A:174:GLU:OE2	1:A:174:GLU:HA	2.09	0.51
1:A:231:MSE:HE3	1:A:233:ASN:HB2	1.92	0.51
1:A:322:MSE:O	1:A:323:ARG:C	2.54	0.51
1:A:286:GLN:NE2	1:A:286:GLN:HA	2.26	0.51
1:A:221:ASN:O	1:A:222:VAL:HG23	2.11	0.51
1:A:286:GLN:HA	1:A:286:GLN:HE21	1.75	0.50
1:A:387:LEU:O	1:A:391:GLU:HG3	2.11	0.50
1:A:30:GLY:O	1:A:33:LYS:HB2	2.12	0.50
1:A:58:LEU:O	1:A:168:ALA:HA	2.12	0.50
1:A:360:GLN:HB3	1:A:364:MSE:CE	2.42	0.49
1:A:31:GLN:OE1	1:A:171:PRO:O	2.29	0.49
1:A:59:MSE:HE1	1:A:186:ALA:HB3	1.93	0.49
1:A:3:LYS:N	3:A:601:SO4:O2	2.39	0.49
1:A:303:LYS:HG2	1:A:304:GLY:N	2.28	0.49
1:A:303:LYS:HD3	1:A:304:GLY:H	1.78	0.49
1:A:47:LEU:HD11	1:A:152:LEU:HD13	1.94	0.48
1:A:324:GLU:O	1:A:328:GLU:HB2	2.13	0.48
1:A:1:MSE:HE2	1:A:394:VAL:CG1	2.44	0.48
1:A:126:GLN:HG2	1:A:388:GLU:HG3	1.94	0.48
1:A:40:GLN:HA	1:A:43:GLU:HG3	1.95	0.48
1:A:190:GLN:HG2	1:A:191:TRP:CE3	2.47	0.48
1:A:74:GLY:HA2	1:A:166:LYS:O	2.12	0.48
1:A:39:LYS:O	1:A:43:GLU:HG2	2.15	0.47
1:A:288:GLU:OE1	1:A:288:GLU:HA	2.14	0.47
1:A:16:THR:HG23	1:A:31:GLN:HG2	1.96	0.47
1:A:281:ASP:OD2	1:A:290:ARG:NH1	2.50	0.45
1:A:286:GLN:O	1:A:290:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLY:O	1:A:303:LYS:C	2.59	0.45
1:A:70:ILE:HG21	1:A:405:ALA:HA	1.98	0.45
1:A:226:THR:HG22	1:A:226:THR:O	2.16	0.45
1:A:134:LYS:HE3	1:A:135:THR:HG23	1.97	0.45
1:A:246:PRO:HB2	1:A:249:GLU:HB2	1.98	0.45
1:A:55:LYS:HA	1:A:55:LYS:HD3	1.69	0.45
1:A:205:PHE:HE1	1:A:349:MSE:HE2	1.81	0.45
1:A:88:LYS:HG3	1:A:89:ASN:N	2.32	0.44
1:A:78:HIS:NE2	1:A:141:ASP:HB2	2.32	0.44
1:A:77:SER:O	1:A:169:PHE:HA	2.16	0.44
1:A:200:VAL:HG23	4:A:618:HOH:O	2.18	0.44
1:A:140:ASP:HA	1:A:141:ASP:HA	1.78	0.44
1:A:208:PHE:CE1	1:A:280:ARG:HB3	2.53	0.44
1:A:288:GLU:O	1:A:292:ARG:HG2	2.17	0.44
1:A:245:VAL:HA	1:A:246:PRO:HD3	1.78	0.43
1:A:223:HIS:CE1	1:A:225:GLY:H	2.37	0.43
1:A:255:GLU:H	1:A:258:GLU:CG	2.32	0.43
1:A:288:GLU:OE1	1:A:291:LYS:HE2	2.18	0.43
1:A:70:ILE:CG2	1:A:405:ALA:HA	2.49	0.43
1:A:254:THR:HB	1:A:258:GLU:HG3	2.01	0.43
1:A:322:MSE:O	1:A:325:LYS:N	2.52	0.43
1:A:333:LEU:O	1:A:337:GLN:HG3	2.19	0.43
1:A:126:GLN:CG	1:A:388:GLU:HG3	2.49	0.43
1:A:143:ALA:HB1	1:A:390:MSE:HE3	2.00	0.43
1:A:85:PHE:HB3	1:A:136:LEU:HG	2.01	0.43
1:A:134:LYS:O	1:A:134:LYS:HG2	2.19	0.42
1:A:283:ASP:OD2	1:A:285:LYS:HB2	2.19	0.42
1:A:12:VAL:HG13	1:A:137:LEU:O	2.19	0.42
1:A:132:ASP:OD2	1:A:134:LYS:N	2.36	0.42
1:A:207:ASN:O	1:A:321:ASN:CG	2.62	0.42
1:A:215:ILE:HA	1:A:312:GLU:O	2.20	0.42
1:A:3:LYS:O	1:A:7:ARG:HG3	2.20	0.42
1:A:16:THR:HG21	1:A:79:VAL:HG13	2.00	0.42
1:A:132:ASP:OD2	1:A:132:ASP:C	2.63	0.42
1:A:138:GLY:O	1:A:142:LYS:HB2	2.20	0.42
1:A:59:MSE:HE1	1:A:186:ALA:HB1	2.00	0.41
1:A:55:LYS:NZ	4:A:637:HOH:O	2.52	0.41
1:A:255:GLU:H	1:A:258:GLU:HG3	1.85	0.41
1:A:222:VAL:CG1	1:A:223:HIS:N	2.84	0.41
1:A:322:MSE:HG2	1:A:359:ALA:CB	2.51	0.41
1:A:47:LEU:HD23	1:A:47:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ALA:HB1	1:A:280:ARG:HH21	1.82	0.41
1:A:96:GLU:HG3	1:A:127:THR:HG23	2.02	0.40
1:A:4:LEU:HD12	1:A:391:GLU:HG2	2.04	0.40
1:A:237:LEU:HD22	1:A:301:VAL:HG12	2.03	0.40
1:A:266:MSE:HA	1:A:274:GLU:O	2.21	0.40
1:A:23:ARG:HD2	1:A:23:ARG:HA	1.89	0.40
1:A:85:PHE:CD1	1:A:135:THR:HA	2.56	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	406/417 (97%)	384 (95%)	15 (4%)	7 (2%)	7 10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	LYS
1	A	307	PRO
1	A	88	LYS
1	A	171	PRO
1	A	323	ARG
1	A	246	PRO
1	A	256	GLY

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	329/328 (100%)	288 (88%)	41 (12%)	4 6

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	4	LEU
1	A	5	LEU
1	A	18	SER
1	A	20	SER
1	A	24	GLN
1	A	43	GLU
1	A	47	LEU
1	A	48	VAL
1	A	52	LEU
1	A	58	LEU
1	A	62	LEU
1	A	67	GLU
1	A	77	SER
1	A	79	VAL
1	A	93	GLN
1	A	97	ASN
1	A	119	VAL
1	A	122	GLN
1	A	137	LEU
1	A	177	LYS
1	A	180	LYS
1	A	184	VAL
1	A	190	GLN
1	A	202	GLU
1	A	203	LEU
1	A	222	VAL
1	A	228	LYS
1	A	263	LEU
1	A	266	MSE
1	A	293	LYS
1	A	307	PRO
1	A	313	LEU
1	A	322	MSE
1	A	324	GLU

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Mol	Chain	Res	Type
1	A	348	GLU
1	A	366	LEU
1	A	371	LEU
1	A	387	LEU
1	A	388	GLU
1	A	399	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	41	GLN
1	A	65	ASN
1	A	93	GLN
1	A	158	ASN
1	A	190	GLN
1	A	214	ASN
1	A	286	GLN
1	A	329	HIS
1	A	331	HIS
1	A	338	GLN
1	A	377	ASN
1	A	379	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	SO4	A	600	-	4,4,4	0.45	0	6,6,6	0.21	0
3	SO4	A	601	-	4,4,4	0.49	0	6,6,6	0.19	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
3	A	601	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	393/417 (94%)	0.14	12 (3%) 51 47	18, 40, 70, 105	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	GLY	4.4
1	A	134	LYS	3.4
1	A	306	HIS	2.9
1	A	378	TYR	2.8
1	A	286	GLN	2.5
1	A	2	ASP	2.4
1	A	171	PRO	2.3
1	A	307	PRO	2.1
1	A	175	VAL	2.1
1	A	272	ARG	2.0
1	A	91	ASN	2.0
1	A	221	ASN	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
3	SO4	A	600	5/5	0.83	0.13	86,86,86,86	0
3	SO4	A	601	5/5	0.85	0.14	80,80,80,80	0
2	ZN	A	502	1/1	0.90	0.12	111,111,111,111	0
2	ZN	A	501	1/1	0.98	0.03	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.