



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:11 AM UTC

PDB ID : 1TE6 / pdb_00001te6
Title : Crystal Structure of Human Neuron Specific Enolase at 1.8 angstrom
Authors : Chai, G.; Brewer, J.; Lovelace, L.; Aoki, T.; Minor, W.; Lebioda, L.
Deposited on : 2004-05-24
Resolution : 1.80 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

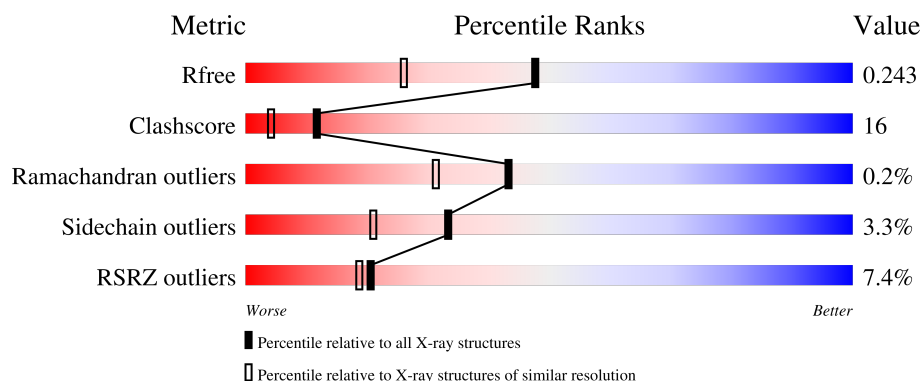
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	439	7% 74% 23% ..
1	B	439	8% 71% 24% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7110 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 Gamma enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3319	2087	569	650	13			
1	B	433	Total	C	N	O	S	0	0	0
			3314	2084	568	649	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	HIS	-	expression tag	UNP P09104
A	435	HIS	-	expression tag	UNP P09104
A	436	HIS	-	expression tag	UNP P09104
A	437	HIS	-	expression tag	UNP P09104
A	438	HIS	-	expression tag	UNP P09104
A	439	HIS	-	expression tag	UNP P09104
B	434	HIS	-	expression tag	UNP P09104
B	435	HIS	-	expression tag	UNP P09104
B	436	HIS	-	expression tag	UNP P09104
B	437	HIS	-	expression tag	UNP P09104
B	438	HIS	-	expression tag	UNP P09104
B	439	HIS	-	expression tag	UNP P09104

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

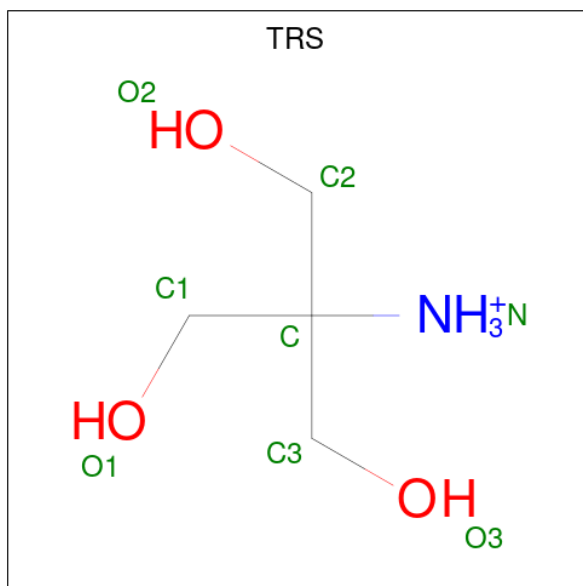
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0

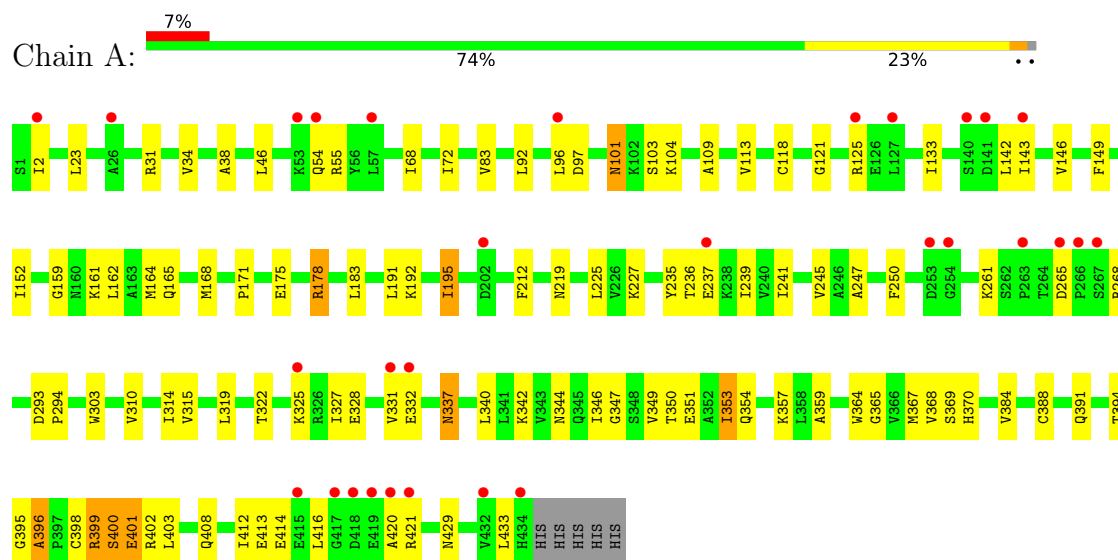
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	236	Total 236	O 236	0	0
6	B	224	Total 224	O 224	0	0

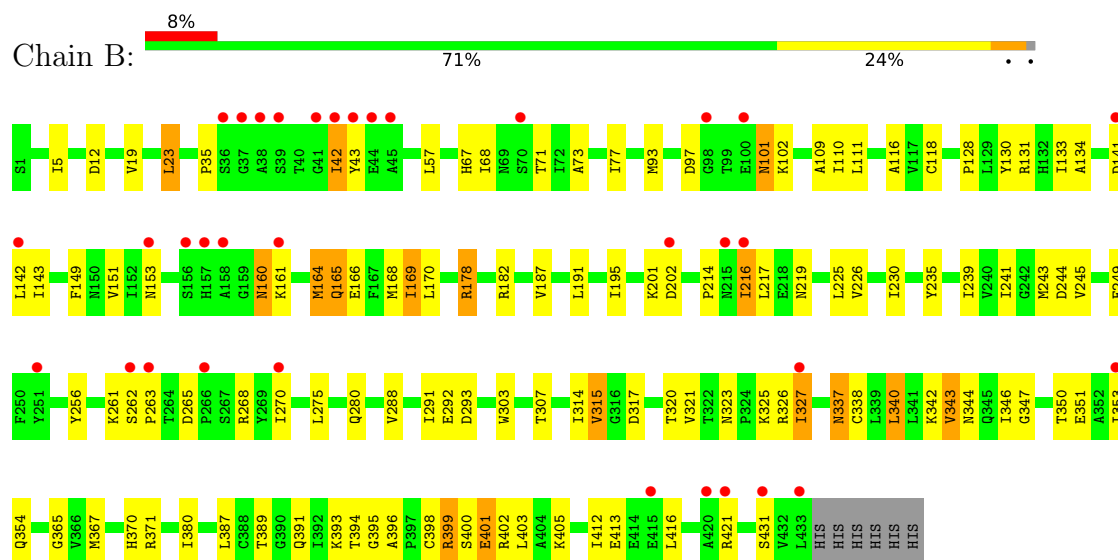
3 Residue-property plots

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: Gamma enolase



• Molecule 1: Gamma enolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.58Å 119.71Å 68.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-1.80) 94.2 (30.00-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.234 0.214 , 0.243	Depositor DCC
R_{free} test set	4157 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7110	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: CL, MG, TRS, PO4

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	0.40	0/3374	0.90	13/4565 (0.3%)
1	B	0.39	0/3369	0.86	11/4558 (0.2%)
All	All	0.39	0/6743	0.88	24/9123 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	GLN	N-CA-C	10.13	122.08	111.14
1	A	146	VAL	N-CA-C	-8.56	101.27	108.63
1	B	165	GLN	N-CA-C	8.26	121.47	111.40
1	A	401	GLU	N-CA-C	-7.88	103.56	113.01
1	A	395	GLY	N-CA-C	7.33	119.52	112.04
1	B	395	GLY	N-CA-C	6.96	120.61	111.70
1	B	396	ALA	N-CA-C	-6.91	99.98	110.07
1	B	401	GLU	N-CA-C	-6.86	104.78	113.01
1	A	396	ALA	N-CA-C	-6.83	100.10	110.07
1	A	34	VAL	N-CA-C	6.38	114.84	107.89
1	B	365	GLY	N-CA-C	-6.30	102.94	112.89
1	A	315	VAL	N-CA-C	6.25	117.29	108.36
1	A	38	ALA	N-CA-C	-6.18	104.71	112.93
1	B	400	SER	N-CA-C	5.96	120.02	112.87
1	A	365	GLY	N-CA-C	-5.86	103.63	112.89
1	A	400	SER	N-CA-C	5.60	119.73	113.01
1	B	340	LEU	N-CA-C	-5.53	100.29	109.46
1	A	241	ILE	N-CA-C	5.52	116.53	108.53
1	B	347	GLY	N-CA-C	5.32	121.84	114.92
1	B	19	VAL	N-CA-C	5.26	116.86	108.87
1	A	369	SER	N-CA-C	5.19	117.28	109.23
1	B	315	VAL	N-CA-C	5.17	115.76	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	GLY	N-CA-C	5.08	121.75	114.64
1	B	343	VAL	N-CA-C	5.01	115.62	110.36

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	3319	0	3291	95	0
1	B	3314	0	3290	119	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
4	A	8	0	12	0	0
5	B	1	0	0	0	0
6	A	236	0	0	3	0
6	B	224	0	0	4	0
All	All	7110	0	6593	210	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 (210) 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:353:ILE:HD12	1:B:387:LEU:HD21	1.16	1.07
1:A:68:ILE:HD13	1:A:72:ILE:HD12	1.38	1.06
1:B:214:PRO:O	1:B:216:ILE:HD13	1.65	0.95
1:B:214:PRO:HG2	1:B:216:ILE:HD12	1.50	0.94
1:A:2:ILE:CD1	1:A:23:LEU:HD21	2.01	0.91
1:B:314:ILE:H	1:B:337:ASN:HD21	1.20	0.86
1:A:349:VAL:O	1:A:353:ILE:HD13	1.76	0.85
1:B:169:ILE:HD13	1:B:169:ILE:H	1.46	0.80
1:B:93:MET:HB3	1:B:110:ILE:HD12	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:MET:HB2	1:B:291:ILE:CD1	2.14	0.78
1:B:323:ASN:O	1:B:327:ILE:HD13	1.85	0.77
1:A:68:ILE:CD1	1:A:72:ILE:HD12	2.15	0.76
1:A:2:ILE:HD13	1:A:23:LEU:HD21	1.68	0.76
1:B:314:ILE:H	1:B:337:ASN:ND2	1.85	0.75
1:B:149:PHE:O	1:B:169:ILE:HD13	1.85	0.75
1:A:68:ILE:HD12	1:A:113:VAL:CG2	2.19	0.73
1:A:314:ILE:H	1:A:337:ASN:HD21	1.35	0.71
1:B:243:MET:HB2	1:B:291:ILE:HD13	1.71	0.71
1:B:214:PRO:O	1:B:216:ILE:CD1	2.38	0.69
1:A:421:ARG:NH1	1:A:433:LEU:HB3	2.08	0.69
1:B:187:VAL:HG11	1:B:230:ILE:HD13	1.74	0.68
1:B:130:TYR:CD2	1:B:412:ILE:HD12	2.29	0.68
1:B:161:LYS:HB3	1:B:217:LEU:HD13	1.76	0.68
1:B:141:ASP:HB3	1:B:421:ARG:HH22	1.57	0.67
1:B:130:TYR:CE2	1:B:412:ILE:HD12	2.29	0.67
1:A:195:ILE:HD12	1:A:225:LEU:HD22	1.77	0.66
1:A:164:MET:HG2	1:A:245:VAL:HG13	1.78	0.66
1:B:151:VAL:HG13	1:B:169:ILE:CD1	2.25	0.66
1:B:353:ILE:CD1	1:B:387:LEU:HD21	2.10	0.66
1:B:164:MET:HB2	1:B:219:ASN:ND2	2.10	0.66
1:B:262:SER:HB3	1:B:263:PRO:HD2	1.78	0.65
1:A:416:LEU:HD13	1:A:420:ALA:HB2	1.77	0.65
1:B:293:ASP:OD2	1:B:317:ASP:HB3	1.96	0.65
1:B:164:MET:HG3	1:B:245:VAL:HG13	1.79	0.64
1:B:214:PRO:HG2	1:B:216:ILE:CD1	2.25	0.64
1:B:178:ARG:HD3	1:B:413:GLU:OE1	1.96	0.64
1:A:353:ILE:HG22	1:A:357:LYS:HE2	1.81	0.63
1:A:118:CYS:SG	1:A:133:ILE:HD11	2.37	0.63
1:B:164:MET:H	1:B:219:ASN:HD21	1.44	0.63
1:B:288:VAL:HG11	1:B:291:ILE:HD11	1.81	0.63
1:B:350:THR:O	1:B:354:GLN:HG3	1.99	0.63
1:B:169:ILE:HD13	1:B:169:ILE:N	2.12	0.63
1:A:164:MET:H	1:A:219:ASN:HD21	1.46	0.63
1:B:149:PHE:HB2	1:B:169:ILE:HD11	1.82	0.62
1:A:314:ILE:H	1:A:337:ASN:ND2	1.96	0.62
1:B:42:ILE:HD13	1:B:42:ILE:N	2.13	0.62
1:A:101:ASN:HD22	1:A:101:ASN:H	1.48	0.62
1:B:256:TYR:HB2	1:B:270:ILE:HD11	1.82	0.61
1:A:2:ILE:HD12	1:A:23:LEU:HD21	1.83	0.61
1:B:151:VAL:HG13	1:B:169:ILE:HD11	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HD12	1:A:113:VAL:HG21	1.81	0.61
1:B:256:TYR:HB2	1:B:270:ILE:CD1	2.31	0.61
1:A:328:GLU:O	1:A:331:VAL:HG22	2.00	0.61
1:A:2:ILE:HD12	1:A:23:LEU:HD11	1.84	0.60
1:A:164:MET:HB2	1:A:219:ASN:ND2	2.17	0.60
1:B:118:CYS:SG	1:B:133:ILE:HD11	2.42	0.59
1:A:46:LEU:HD23	1:A:103:SER:HA	1.85	0.59
1:B:270:ILE:CD1	1:B:275:LEU:HB2	2.33	0.59
1:B:337:ASN:C	1:B:337:ASN:HD22	2.10	0.59
1:A:178:ARG:HD3	1:A:413:GLU:OE1	2.03	0.59
1:B:165:GLN:HG2	1:B:166:GLU:HG3	1.84	0.58
1:A:236:THR:HG22	1:A:237:GLU:HG3	1.84	0.58
1:B:398:CYS:O	1:B:399:ARG:HB2	2.03	0.58
1:A:191:LEU:O	1:A:195:ILE:HD13	2.03	0.58
1:A:178:ARG:HH21	1:A:414:GLU:HB2	1.69	0.57
1:B:101:ASN:H	1:B:101:ASN:HD22	1.51	0.57
1:B:270:ILE:HD13	1:B:275:LEU:HB2	1.85	0.57
1:B:320:THR:HB	1:B:327:ILE:CD1	2.35	0.57
1:A:421:ARG:NH1	1:A:421:ARG:HB3	2.19	0.57
1:B:346:ILE:HG12	1:B:351:GLU:HB3	1.86	0.57
1:B:111:LEU:HD22	1:B:344:ASN:HA	1.87	0.56
1:A:68:ILE:HD12	1:A:113:VAL:HG23	1.88	0.56
1:A:2:ILE:HD11	1:A:83:VAL:HG12	1.87	0.56
1:A:101:ASN:H	1:A:101:ASN:ND2	2.04	0.55
1:A:92:LEU:O	1:A:96:LEU:HG	2.06	0.55
1:B:149:PHE:HB2	1:B:169:ILE:CD1	2.37	0.55
1:A:159:GLY:O	1:B:202:ASP:HA	2.07	0.55
1:A:370:HIS:CG	1:A:394:THR:HA	2.42	0.55
1:A:183:LEU:HD22	1:A:235:TYR:CZ	2.42	0.55
1:A:367:MET:HA	1:A:391:GLN:HG3	1.89	0.55
1:A:101:ASN:HD22	1:A:101:ASN:N	2.03	0.54
1:A:143:ILE:O	1:A:143:ILE:HD12	2.06	0.54
1:B:307:THR:HG23	1:B:314:ILE:HD13	1.89	0.54
1:B:243:MET:HB2	1:B:291:ILE:HD12	1.87	0.54
1:A:171:PRO:HA	1:A:239:ILE:HD13	1.90	0.54
1:A:261:LYS:HB3	1:B:201:LYS:HE3	1.89	0.54
1:A:340:LEU:CD2	1:A:342:LYS:HE3	2.37	0.53
1:A:337:ASN:C	1:A:337:ASN:HD22	2.17	0.53
1:B:244:ASP:HA	1:B:292:GLU:HB3	1.90	0.52
1:B:151:VAL:CG1	1:B:169:ILE:CD1	2.88	0.52
1:A:68:ILE:HD11	1:A:109:ALA:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:HIS:CD2	1:A:370:HIS:H	2.28	0.52
1:B:320:THR:HB	1:B:327:ILE:HD12	1.91	0.52
1:B:73:ALA:O	1:B:77:ILE:HG13	2.09	0.51
1:B:151:VAL:CG1	1:B:169:ILE:HD11	2.41	0.51
1:B:195:ILE:HD11	1:B:225:LEU:HD13	1.93	0.51
1:B:5:ILE:HG12	1:B:23:LEU:HD22	1.91	0.50
1:A:195:ILE:CD1	1:A:195:ILE:N	2.74	0.50
1:B:160:ASN:C	1:B:160:ASN:HD22	2.20	0.50
1:B:187:VAL:HG11	1:B:230:ILE:CD1	2.40	0.50
1:B:340:LEU:HD23	1:B:342:LYS:HE3	1.92	0.50
1:A:310:VAL:HG21	1:A:314:ILE:HD11	1.94	0.50
1:A:236:THR:O	1:A:237:GLU:HB2	2.12	0.50
1:A:398:CYS:O	1:A:399:ARG:HB2	2.11	0.49
1:A:68:ILE:HD11	1:A:109:ALA:C	2.38	0.49
1:B:57:LEU:N	1:B:57:LEU:HD12	2.27	0.49
1:B:164:MET:HB2	1:B:219:ASN:HD22	1.74	0.49
1:A:340:LEU:HD23	1:A:342:LYS:HE3	1.93	0.49
1:B:187:VAL:CG1	1:B:230:ILE:HD13	2.41	0.49
1:A:247:ALA:HA	1:A:250:PHE:CE1	2.48	0.49
1:B:235:TYR:HB2	1:B:239:ILE:HD12	1.95	0.49
1:B:265:ASP:O	1:B:268:ARG:HG2	2.12	0.48
1:A:2:ILE:HD11	1:A:83:VAL:CG1	2.43	0.48
1:B:142:LEU:C	1:B:143:ILE:HG13	2.39	0.48
1:B:142:LEU:HD22	1:B:142:LEU:H	1.78	0.48
1:B:327:ILE:CD1	1:B:327:ILE:N	2.76	0.48
1:B:128:PRO:HG2	1:B:131:ARG:HB2	1.95	0.48
1:B:293:ASP:HA	1:B:303:TRP:CH2	2.48	0.48
1:A:118:CYS:SG	1:A:133:ILE:CD1	3.01	0.48
1:A:2:ILE:CD1	1:A:23:LEU:HD11	2.43	0.48
1:A:149:PHE:O	1:A:168:MET:HA	2.14	0.48
1:A:152:ILE:HD13	1:A:212:PHE:HB2	1.95	0.48
1:B:340:LEU:HD11	1:B:393:LYS:HE2	1.95	0.48
1:A:322:THR:O	1:A:322:THR:HG22	2.14	0.47
1:A:293:ASP:HA	1:A:303:TRP:CH2	2.49	0.47
1:B:23:LEU:HB2	1:B:116:ALA:HB1	1.96	0.47
1:B:67:HIS:O	1:B:71:THR:HB	2.14	0.47
1:B:226:VAL:HG11	1:B:241:ILE:HD12	1.95	0.47
1:A:31:ARG:HD2	6:A:883:HOH:O	2.15	0.47
1:B:216:ILE:HD13	1:B:216:ILE:H	1.79	0.47
1:A:350:THR:O	1:A:354:GLN:HG3	2.14	0.47
1:B:216:ILE:HD13	1:B:216:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ASN:OD1	1:B:325:LYS:HE2	2.15	0.47
1:A:294:PRO:HD2	1:A:303:TRP:CH2	2.50	0.46
1:B:261:LYS:HB2	6:B:775:HOH:O	2.14	0.46
1:A:143:ILE:HD12	1:A:143:ILE:C	2.41	0.46
1:A:125:ARG:HD2	6:A:978:HOH:O	2.15	0.46
1:B:370:HIS:CG	1:B:394:THR:HA	2.51	0.46
1:B:130:TYR:HE1	1:B:131:ARG:NH1	2.14	0.46
1:B:370:HIS:CD2	1:B:370:HIS:H	2.33	0.46
1:A:161:LYS:O	1:A:162:LEU:C	2.59	0.45
1:B:401:GLU:HG2	1:B:402:ARG:NE	2.31	0.45
1:A:353:ILE:CD1	1:A:353:ILE:N	2.79	0.45
1:A:83:VAL:HG23	1:A:121:GLY:HA2	1.97	0.45
1:B:101:ASN:HD22	1:B:101:ASN:N	2.11	0.45
1:A:396:ALA:C	1:A:398:CYS:H	2.25	0.45
1:B:380:ILE:HD11	1:B:405:LYS:HG2	1.99	0.45
1:B:393:LYS:O	1:B:393:LYS:HG3	2.17	0.45
1:B:141:ASP:HB3	1:B:421:ARG:NH2	2.30	0.45
1:A:54:GLN:HA	1:A:54:GLN:HE21	1.82	0.44
1:B:327:ILE:HD13	1:B:327:ILE:N	2.33	0.44
1:B:340:LEU:CD2	1:B:342:LYS:HE3	2.47	0.44
1:A:328:GLU:O	1:A:332:GLU:HG2	2.17	0.44
1:B:131:ARG:HH12	1:B:416:LEU:HD21	1.82	0.44
1:A:408:GLN:O	1:A:412:ILE:HG13	2.18	0.44
1:A:101:ASN:ND2	1:A:101:ASN:N	2.65	0.44
1:A:191:LEU:CD1	1:A:195:ILE:HD11	2.47	0.44
1:A:265:ASP:O	1:A:268:ARG:HG2	2.17	0.44
1:A:54:GLN:HA	1:A:54:GLN:NE2	2.33	0.44
1:A:191:LEU:HD11	1:A:195:ILE:HD11	2.00	0.44
1:A:359:ALA:O	1:A:364:TRP:HB2	2.18	0.44
1:B:134:ALA:HB2	1:B:142:LEU:HD11	2.00	0.44
1:B:149:PHE:O	1:B:168:MET:HA	2.18	0.44
1:A:331:VAL:HG12	1:A:364:TRP:CZ2	2.53	0.44
1:B:101:ASN:H	1:B:101:ASN:ND2	2.15	0.44
1:B:169:ILE:HG22	1:B:241:ILE:CD1	2.48	0.44
1:A:325:LYS:O	1:A:325:LYS:HD3	2.18	0.43
1:B:320:THR:HB	1:B:327:ILE:HD11	2.00	0.43
1:B:367:MET:HA	1:B:391:GLN:HG3	1.99	0.43
1:A:171:PRO:HA	1:A:239:ILE:CD1	2.49	0.43
1:A:325:LYS:HD3	1:A:325:LYS:C	2.44	0.43
1:A:346:ILE:HG12	1:A:351:GLU:HB3	2.00	0.43
1:B:270:ILE:HD12	1:B:270:ILE:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLU:HG2	1:A:402:ARG:NE	2.34	0.43
1:B:230:ILE:HD12	1:B:239:ILE:HG21	1.99	0.43
1:B:153:ASN:ND2	6:B:780:HOH:O	2.52	0.43
1:A:368:VAL:HG21	1:A:384:VAL:HA	2.01	0.43
1:B:169:ILE:CD1	1:B:169:ILE:N	2.81	0.42
1:A:97:ASP:O	1:A:104:LYS:HE2	2.18	0.42
1:A:421:ARG:HH12	1:A:433:LEU:HD13	1.85	0.42
1:B:323:ASN:HB3	1:B:326:ARG:HG3	2.01	0.42
1:A:327:ILE:O	1:A:331:VAL:HG13	2.19	0.42
1:B:249:GLU:HG3	6:B:752:HOH:O	2.18	0.42
1:B:118:CYS:SG	1:B:133:ILE:CD1	3.06	0.42
1:B:230:ILE:CD1	1:B:239:ILE:HG21	2.49	0.42
1:B:68:ILE:HD11	1:B:109:ALA:HA	2.00	0.42
1:A:55:ARG:HG3	1:B:182:ARG:HD2	2.00	0.42
1:B:343:VAL:O	1:B:346:ILE:HG22	2.20	0.42
1:B:161:LYS:HD2	1:B:161:LYS:N	2.34	0.41
1:B:195:ILE:CD1	1:B:225:LEU:HD13	2.50	0.41
1:A:400:SER:HB2	1:B:401:GLU:HB3	2.02	0.41
1:B:43:TYR:HB2	1:B:321:VAL:HG21	2.01	0.41
1:A:142:LEU:HA	1:A:388:CYS:SG	2.60	0.41
1:B:169:ILE:C	1:B:170:LEU:HD12	2.45	0.41
1:B:164:MET:H	1:B:219:ASN:ND2	2.16	0.41
1:A:192:LYS:HB2	1:A:212:PHE:CZ	2.54	0.41
1:A:227:LYS:HD3	1:A:227:LYS:O	2.20	0.41
1:B:97:ASP:OD2	1:B:102:LYS:HA	2.20	0.41
1:B:42:ILE:N	1:B:42:ILE:CD1	2.78	0.41
1:A:340:LEU:HD21	1:A:342:LYS:HE3	2.03	0.41
1:B:12:ASP:OD1	1:B:12:ASP:C	2.64	0.41
1:B:314:ILE:N	1:B:337:ASN:HD21	2.00	0.41
1:A:183:LEU:CD1	1:A:239:ILE:HD11	2.51	0.40
1:A:303:TRP:CD2	1:A:319:LEU:HD22	2.56	0.40
1:B:315:VAL:HG22	1:B:338:CYS:HB3	2.03	0.40
1:B:398:CYS:O	1:B:399:ARG:CB	2.67	0.40
1:B:35:PRO:HB2	1:B:371:ARG:HB2	2.03	0.40
1:A:429:ASN:HB3	6:A:809:HOH:O	2.20	0.40
1:A:314:ILE:N	1:A:337:ASN:HD21	2.13	0.40
1:B:161:LYS:HD3	6:B:931:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	432/439 (98%)	415 (96%)	16 (4%)	1 (0%)	43	31
1	B	431/439 (98%)	414 (96%)	16 (4%)	1 (0%)	43	31
All	All	863/878 (98%)	829 (96%)	32 (4%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	399	ARG
1	A	399	ARG

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	350/356 (98%)	342 (98%)	8 (2%)	44	33
1	B	350/356 (98%)	335 (96%)	15 (4%)	26	13
All	All	700/712 (98%)	677 (97%)	23 (3%)	33	21

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	175	GLU
1	A	178	ARG
1	A	195	ILE

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Mol	Chain	Res	Type
1	A	337	ASN
1	A	344	ASN
1	A	353	ILE
1	A	403	LEU
1	B	23	LEU
1	B	42	ILE
1	B	101	ASN
1	B	160	ASN
1	B	164	MET
1	B	169	ILE
1	B	178	ARG
1	B	191	LEU
1	B	216	ILE
1	B	280	GLN
1	B	327	ILE
1	B	337	ASN
1	B	389	THR
1	B	403	LEU
1	B	431	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	101	ASN
1	A	139	ASN
1	A	150	ASN
1	A	153	ASN
1	A	205	ASN
1	A	219	ASN
1	A	337	ASN
1	A	360	GLN
1	A	426	ASN
1	B	91	ASN
1	B	101	ASN
1	B	135	GLN
1	B	153	ASN
1	B	160	ASN
1	B	215	ASN
1	B	219	ASN
1	B	297	GLN
1	B	337	ASN

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Mol	Chain	Res	Type
1	B	345	GLN
1	B	354	GLN
1	B	360	GLN
1	B	425	HIS
1	B	426	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](#)

Of 6 ligands modelled in this entry, 4 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	$\# Z > 2$
4	TRS	A	660	-	7,7,7	0.86	0	9,9,9	1.79	2 (22%)
3	PO4	A	642	2	4,4,4	1.72	2 (50%)	6,6,6	0.48	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
4	TRS	A	660	-	-	6/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	642	PO4	P-O2	-2.12	1.48	1.54
3	A	642	PO4	P-O4	-2.02	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	660	TRS	C2-C-N	4.18	118.83	108.17
4	A	660	TRS	C1-C-N	-2.07	102.90	108.17

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	660	TRS	C1-C-C2-O2
4	A	660	TRS	C3-C-C2-O2
4	A	660	TRS	C1-C-C3-O3
4	A	660	TRS	C2-C-C3-O3
4	A	660	TRS	N-C-C2-O2
4	A	660	TRS	N-C-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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

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	434/439 (98%)	0.24	30 (6%) 23 21	15, 23, 42, 63	0
1	B	433/439 (98%)	0.46	34 (7%) 18 16	15, 25, 47, 59	0
All	All	867/878 (98%)	0.35	64 (7%) 20 19	15, 24, 45, 63	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	ASP	6.9
1	B	100	GLU	6.5
1	B	157	HIS	6.1
1	B	158	ALA	5.8
1	A	54	GLN	5.6
1	A	253	ASP	5.3
1	A	419	GLU	5.2
1	A	420	ALA	4.6
1	B	42	ILE	4.1
1	B	431	SER	4.1
1	B	43	TYR	4.0
1	A	421	ARG	3.9
1	A	332	GLU	3.9
1	A	143	ILE	3.5
1	B	38	ALA	3.5
1	B	263	PRO	3.4
1	B	262	SER	3.3
1	B	41	GLY	3.2
1	B	156	SER	3.1
1	A	125	ARG	3.1
1	B	161	LYS	3.1
1	B	270	ILE	3.1
1	A	434	HIS	3.1
1	B	433	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	263	PRO	3.0
1	A	265	ASP	2.9
1	B	202	ASP	2.9
1	B	44	GLU	2.8
1	B	142	LEU	2.8
1	B	36	SER	2.8
1	A	237	GLU	2.7
1	A	2	ILE	2.7
1	B	421	ARG	2.7
1	A	415	GLU	2.7
1	B	98	GLY	2.7
1	B	216	ILE	2.6
1	A	254	GLY	2.6
1	B	37	GLY	2.6
1	A	417	GLY	2.5
1	B	39	SER	2.5
1	A	325	LYS	2.5
1	B	420	ALA	2.5
1	A	57	LEU	2.5
1	A	331	VAL	2.5
1	B	415	GLU	2.4
1	B	215	ASN	2.4
1	A	267	SER	2.4
1	A	140	SER	2.3
1	A	127	LEU	2.3
1	B	45	ALA	2.3
1	B	70	SER	2.3
1	A	96	LEU	2.2
1	B	153	ASN	2.2
1	A	266	PRO	2.2
1	A	141	ASP	2.2
1	A	202	ASP	2.2
1	B	141	ASP	2.2
1	A	26	ALA	2.1
1	A	432	VAL	2.1
1	A	53	LYS	2.0
1	B	327	ILE	2.0
1	B	266	PRO	2.0
1	B	353	ILE	2.0
1	B	251	TYR	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
4	TRS	A	660	8/8	0.78	0.26	49,56,57,59	0
3	PO4	A	642	5/5	0.87	0.13	20,21,32,34	0
5	CL	B	742	1/1	0.88	0.12	46,46,46,46	0
2	MG	A	641	1/1	0.93	0.07	17,17,17,17	0
2	MG	A	640	1/1	0.96	0.04	21,21,21,21	0
2	MG	B	740	1/1	0.99	0.02	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.