WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 06:51 am GMT

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PDB ID	:	1TE6
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)

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	Percentile Ranks	Value
Rfree		0.243
Clashscore		16
Ramachandran outliers		0.2%
Sidechain outliers		3.3%
RSRZ outliers		4.6%

Worse — *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
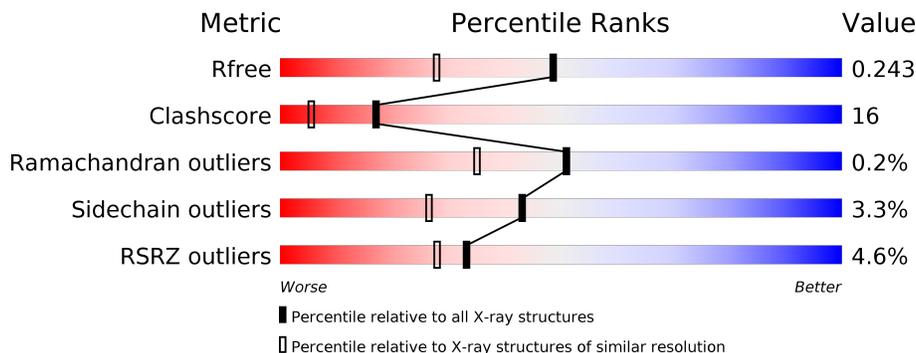
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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 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 <=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	4% — 76% green, 21% yellow ··
1	B	439	5% — 73% green, 23% yellow ··

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
5	TRS	A	660	-	-	-	X

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
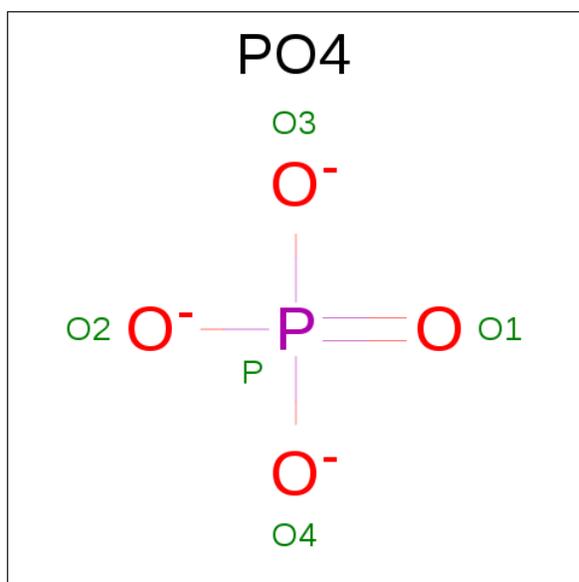
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).
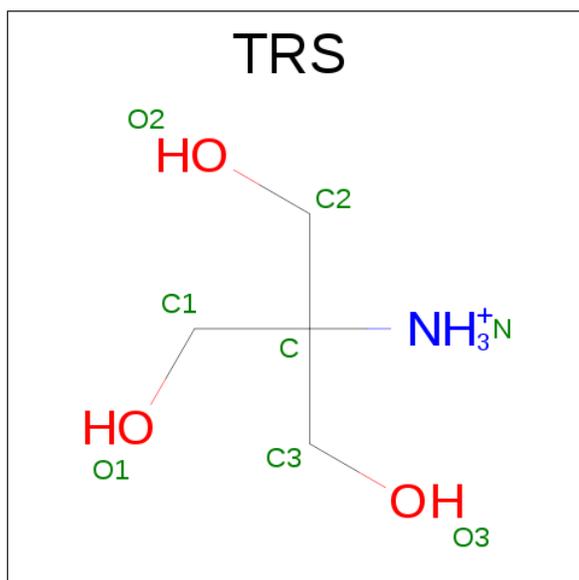
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 8	C 4	N 1	O 3	0	0

- 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 and DNA 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
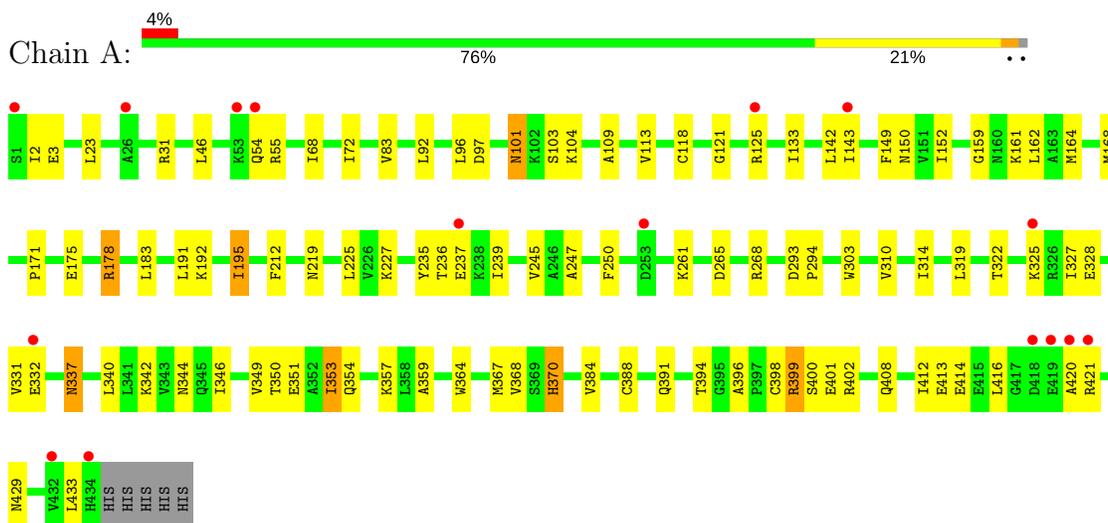
4 Data and refinement statistics ⓘ

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 23.62 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-1.80) 94.2 (23.62-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.04%)	DCC
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 , 47.2	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: TRS, MG, PO4, CL

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	0.36	1/3374 (0.0%)	0.59	0/4565
1	B	0.35	1/3369 (0.0%)	0.58	0/4558
All	All	0.35	2/6743 (0.0%)	0.58	0/9123

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	GLU	CD-OE2	7.11	1.33	1.25
1	B	3	GLU	CD-OE2	7.11	1.33	1.25

There are no bond angle outliers.

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	94	0
1	B	3314	0	3290	116	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
4	B	1	0	0	0	0
5	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	236	0	0	3	0
6	B	224	0	0	4	0
All	All	7110	0	6593	206	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 (206) 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:H	1:B:169:ILE:HD13	1.46	0.80
1:B:93:MET:HB3	1:B:110:ILE:HD12	1.64	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:214:PRO:HG2	1:B:216:ILE:CD1	2.25	0.64
1:B:164:MET:HG3	1:B:245:VAL:HG13	1.79	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
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: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:HB3	1:A:421:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:370:HIS:CG	1:A:394:THR:HA	2.42	0.55
1:A:159:GLY:O	1:B:202:ASP:HA	2.07	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:N	1:A:101:ASN:HD22	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:B:337:ASN:HD22	1:B:337:ASN:C	2.10	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: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
1:A:370:HIS:H	1:A:370:HIS:CD2	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:N	1:A:195:ILE:CD1	2.74	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:B:164:MET:HB2	1:B:219:ASN:HD22	1.74	0.49
1:B:57:LEU:N	1:B:57:LEU:HD12	2.27	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:A:337:ASN:C	1:A:337:ASN:HD22	2.17	0.48
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:HD22	1:B:142:LEU:H	1.78	0.48
1:B:327:ILE:N	1:B:327:ILE:CD1	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:2:ILE:CD1	1:A:23:LEU:HD11	2.43	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:H	1:B:216:ILE:HD13	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
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: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:B:401:GLU:HG2	1:B:402:ARG:NE	2.31	0.45
1:A:353:ILE:N	1:A:353:ILE:CD1	2.79	0.45
1:A:83:VAL:HG23	1:A:121:GLY:HA2	1.97	0.45
1:B:101:ASN:N	1:B:101:ASN:HD22	2.11	0.45
1:B:380:ILE:HD11	1:B:405:LYS:HG2	1.99	0.45
1:A:68:ILE:HD11	1:A:109:ALA:C	2.38	0.45
1:B:393:LYS:HG3	1:B:393:LYS:O	2.17	0.45
1:B:141:ASP:HB3	1:B:421:ARG:NH2	2.30	0.45
1:B:160:ASN:HD22	1:B:160:ASN:C	2.20	0.45
1:A:54:GLN:HE21	1:A:54:GLN:HA	1.82	0.44
1:B:327:ILE:N	1:B:327:ILE:HD13	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:N	1:A:101:ASN:ND2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:54:GLN:NE2	1:A:54:GLN:HA	2.33	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:142:LEU:C	1:B:143:ILE:HG13	2.39	0.44
1:B:169:ILE:HG22	1:B:241:ILE:CD1	2.48	0.44
1:A:325:LYS:HD3	1:A:325:LYS:O	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:346:ILE:HG12	1:A:351:GLU:HB3	2.00	0.43
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:143:ILE:C	1:A:143:ILE:HD12	2.41	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: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:CD1	1:B:42:ILE:N	2.78	0.41
1:A:161:LYS:O	1:A:162:LEU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD21	1:A:342:LYS:HE3	2.03	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:A:396:ALA:C	1:A:398:CYS:H	2.25	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%)	51	35
1	B	431/439 (98%)	414 (96%)	16 (4%)	1 (0%)	51	35
All	All	863/878 (98%)	829 (96%)	32 (4%)	2 (0%)	51	35

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%)	341 (97%)	9 (3%)	51	36
1	B	350/356 (98%)	336 (96%)	14 (4%)	36	19
All	All	700/712 (98%)	677 (97%)	23 (3%)	43	26

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

Mol	Chain	Res	Type
1	A	101	ASN
1	A	150	ASN
1	A	175	GLU
1	A	178	ARG
1	A	195	ILE
1	A	337	ASN
1	A	344	ASN
1	A	353	ILE
1	A	370	HIS
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	370	HIS
1	B	389	THR
1	B	431	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	219	ASN
1	A	309	ASN
1	A	337	ASN
1	A	360	GLN
1	A	426	ASN
1	B	91	ASN
1	B	101	ASN
1	B	153	ASN
1	B	160	ASN
1	B	215	ASN
1	B	219	ASN
1	B	337	ASN
1	B	345	GLN
1	B	360	GLN

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 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	$\#|Z| > 2$
3	PO4	A	642	2	4,4,4	1.35	0	6,6,6	0.40	0
5	TRS	A	660	-	7,7,7	0.93	0	9,9,9	2.09	2 (22%)

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
3	PO4	A	642	2	-	0/0/0/0	0/0/0/0
5	TRS	A	660	-	-	0/9/9/9	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	660	TRS	C1-C-N	-2.27	102.90	107.73
5	A	660	TRS	C2-C-N	5.22	118.83	107.73

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.

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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%)	0.14	16 (3%)	42	37	15, 23, 42, 63	0
1	B	433/439 (98%)	0.28	24 (5%)	26	21	15, 25, 47, 59	0
All	All	867/878 (98%)	0.21	40 (4%)	33	28	15, 24, 45, 63	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	GLN	6.5
1	B	42	ILE	6.3
1	A	253	ASP	6.1
1	B	100	GLU	6.0
1	A	418	ASP	5.8
1	A	419	GLU	5.7
1	B	157	HIS	5.4
1	B	41	GLY	4.3
1	A	421	ARG	4.0
1	B	263	PRO	3.9
1	B	141	ASP	3.8
1	B	158	ALA	3.6
1	A	53	LYS	3.4
1	B	40	THR	3.3
1	B	433	LEU	3.3
1	A	325	LYS	3.3
1	B	161	LYS	3.2
1	B	418	ASP	3.1
1	A	237	GLU	3.1
1	A	332	GLU	3.1
1	A	420	ALA	3.1
1	B	156	SER	3.0
1	A	434	HIS	2.9
1	B	26	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	262	SER	2.8
1	B	39	SER	2.8
1	B	421	ARG	2.7
1	A	125	ARG	2.7
1	A	143	ILE	2.6
1	B	43	TYR	2.6
1	B	38	ALA	2.6
1	B	237	GLU	2.6
1	A	26	ALA	2.5
1	B	159	GLY	2.2
1	B	215	ASN	2.2
1	B	36	SER	2.1
1	A	432	VAL	2.1
1	B	420	ALA	2.1
1	A	1	SER	2.0
1	B	267	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
5	TRS	A	660	8/8	0.72	0.21	7.41	49,56,57,59	0
3	PO4	A	642	5/5	0.91	0.12	1.42	20,21,32,34	0
2	MG	A	641	1/1	0.96	0.07	-1.07	17,17,17,17	0
2	MG	A	640	1/1	0.98	0.09	-1.54	21,21,21,21	0
2	MG	B	740	1/1	0.98	0.03	-5.31	21,21,21,21	0
4	CL	B	742	1/1	0.86	0.12	-	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.