Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 09:53 AM EDT

PDB ID	:	2AKM
Title	:	Fluoride Inhibition of Enolase: Crystal Structure of the Inhibitory Complex
Authors	:	Qin, J.; Chai, G.; Brewer, J.M.; Lovelace, L.L.
Deposited on	:	2005-08-03
Resolution	:	1.92 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 (i) 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 (i)) were used in the production of this report:

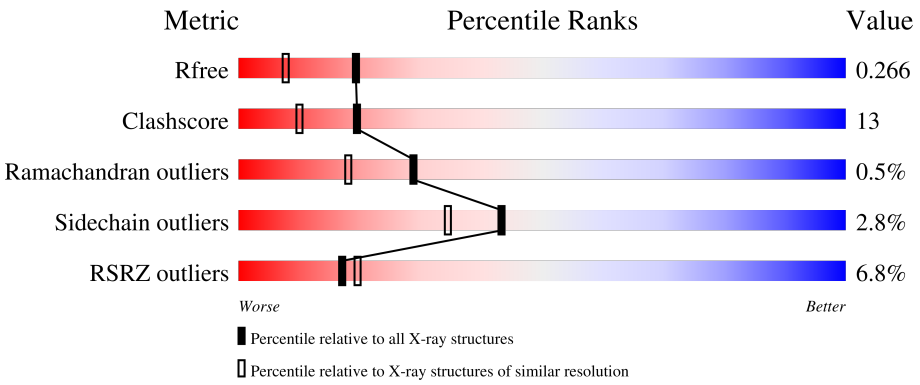
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 <=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	8% 75% 22%
1	B	439	5% 74% 22%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6948 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
			Total	C	N	O	S			
1	A	433	3273	2066	557	637	13	0	0	0
1	B	432	3277	2065	560	639	13	0	0	0

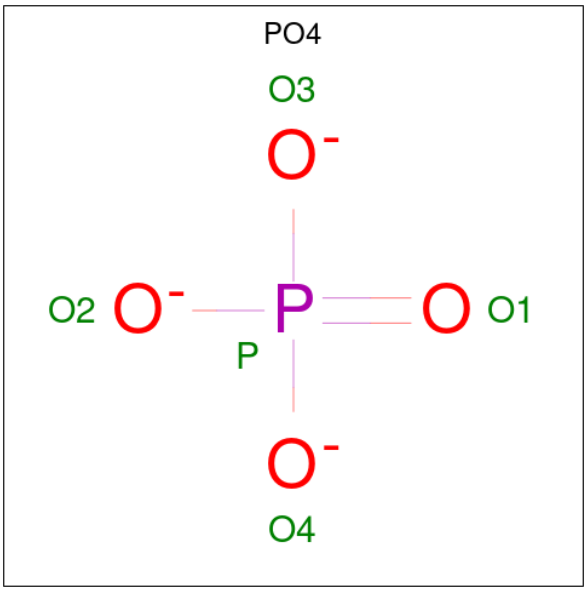
There are 12 discrepancies between the modelled and reference sequences:

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).

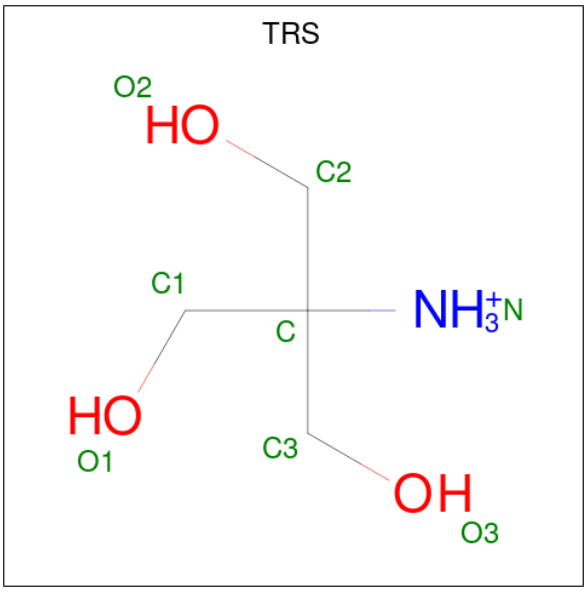
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	2	2	2	0	0
2	B	1	1	1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 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
			Total	C	N	O		
4	A	1	8	4	1	3	0	0

- Molecule 5 is water.

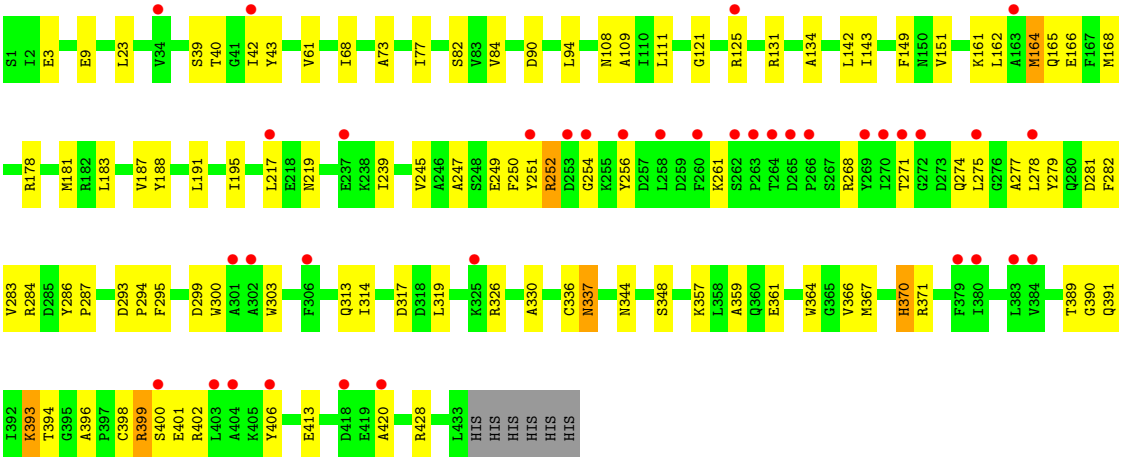
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	186	186	186	0	0
			Total	O		
5	B	191	191	191	0	0

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.

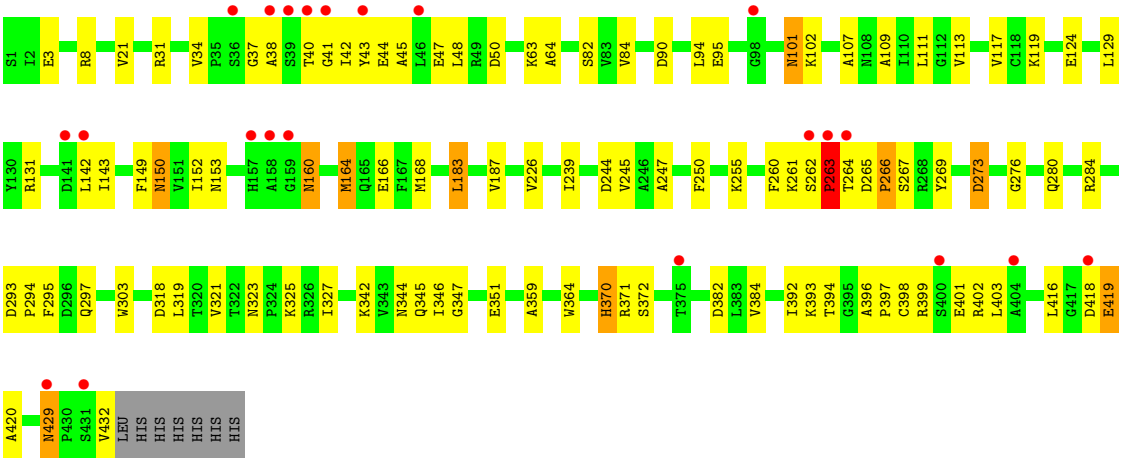
- Molecule 1: Gamma enolase

Chain A:



- Molecule 1: Gamma enolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.74Å 119.69Å 68.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.92 41.75 – 1.92	Depositor EDS
% Data completeness (in resolution range)	74.7 (50.00-1.92) 74.8 (41.75-1.92)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.92Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.249 0.231 , 0.266	Depositor DCC
R_{free} test set	2648 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	1.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6948	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4, TRS

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	0.37	1/3328 (0.0%)	0.57	0/4509
1	B	0.38	1/3332 (0.0%)	0.58	0/4513
All	All	0.38	2/6660 (0.0%)	0.58	0/9022

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	GLU	CD-OE2	7.17	1.33	1.25
1	B	3	GLU	CD-OE2	6.82	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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3273	0	3208	81	0
1	B	3277	0	3225	88	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	8	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	186	0	0	6	0
5	B	191	0	0	8	0
All	All	6948	0	6445	167	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 13.

All (167) 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:273:ASP:HB3	5:B:533:HOH:O	1.81	0.80
1:B:429:ASN:HD22	1:B:429:ASN:N	1.84	0.75
1:B:429:ASN:HD22	1:B:429:ASN:H	1.34	0.73
1:B:342:LYS:NZ	3:B:442:PO4:O2	2.18	0.72
1:B:40:THR:HG22	1:B:371:ARG:HH12	1.56	0.70
1:B:131:ARG:HE	1:B:142:LEU:HD11	1.58	0.69
1:A:164:MET:HB2	1:A:219:ASN:ND2	2.09	0.68
1:A:40:THR:HG22	1:A:371:ARG:HH22	1.59	0.67
1:A:293:ASP:OD2	1:A:317:ASP:HB3	1.95	0.67
1:A:111:LEU:HD22	1:A:344:ASN:HA	1.78	0.65
1:A:357:LYS:O	1:A:361:GLU:HG3	1.96	0.65
1:A:250:PHE:HA	1:A:252:ARG:HH21	1.62	0.65
1:A:261:LYS:HB2	5:A:505:HOH:O	1.96	0.64
1:B:84:VAL:HG13	1:B:124:GLU:HG2	1.80	0.63
1:A:268:ARG:HG3	1:A:268:ARG:HH21	1.64	0.62
1:A:165:GLN:HG2	1:A:166:GLU:HG3	1.81	0.62
1:B:34:VAL:HG13	1:B:111:LEU:HD23	1.81	0.62
1:A:142:LEU:HD22	1:A:142:LEU:H	1.65	0.62
1:A:393:LYS:O	1:A:393:LYS:HG3	2.00	0.61
1:A:247:ALA:HA	1:A:250:PHE:CE1	2.36	0.60
1:B:342:LYS:HB2	1:B:345:GLN:HE21	1.67	0.60
1:B:101:ASN:HD22	1:B:101:ASN:H	1.49	0.59
1:B:266:PRO:HA	1:B:269:TYR:CE2	2.37	0.59
1:A:68:ILE:HD11	1:A:109:ALA:HA	1.84	0.59
1:A:281:ASP:HA	1:A:284:ARG:HH11	1.67	0.59
1:B:152:ILE:HD12	1:B:226:VAL:HG23	1.84	0.58
1:B:44:GLU:HB3	1:B:345:GLN:HG2	1.86	0.57
1:B:342:LYS:HB2	1:B:345:GLN:NE2	2.19	0.57
1:B:94:LEU:CD2	1:B:102:LYS:HE3	2.35	0.57
1:B:164:MET:HG2	1:B:245:VAL:HG22	1.85	0.57
1:A:143:ILE:HD11	1:A:390:GLY:HA2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:MET:HA	1:A:391:GLN:HG3	1.86	0.56
1:B:143:ILE:HD12	1:B:143:ILE:O	2.04	0.56
1:A:247:ALA:HA	1:A:250:PHE:CZ	2.40	0.56
1:B:359:ALA:O	1:B:364:TRP:HB2	2.05	0.56
1:B:41:GLY:O	1:B:44:GLU:HG2	2.06	0.56
1:A:314:ILE:H	1:A:337:ASN:HD21	1.54	0.55
1:A:151:VAL:HG12	1:A:188:TYR:HD1	1.71	0.55
1:A:398:CYS:O	1:A:399:ARG:HB2	2.07	0.55
1:B:82:SER:OG	1:B:84:VAL:HG22	2.06	0.55
1:A:181:MET:CE	1:A:406:TYR:HB3	2.36	0.55
1:A:279:TYR:O	1:A:283:VAL:HG23	2.07	0.55
1:B:398:CYS:O	1:B:399:ARG:HB2	2.07	0.55
1:A:300:TRP:HZ2	1:A:326:ARG:NH2	2.05	0.55
1:B:64:ALA:HB1	1:B:109:ALA:HB2	1.89	0.54
1:A:400:SER:OG	1:B:401:GLU:HB3	2.08	0.54
1:B:131:ARG:HG3	1:B:131:ARG:HH21	1.72	0.54
1:A:164:MET:HG3	1:A:245:VAL:HG13	1.88	0.53
1:A:161:LYS:HB3	1:A:217:LEU:HD13	1.89	0.53
1:B:90:ASP:O	1:B:94:LEU:HG	2.08	0.53
1:B:101:ASN:HD22	1:B:101:ASN:N	2.06	0.53
1:B:160:ASN:HD22	1:B:261:LYS:HZ2	1.54	0.53
1:A:9:GLU:HG3	1:A:61:VAL:CG2	2.39	0.53
1:A:42:ILE:HG13	1:A:43:TYR:CD1	2.44	0.52
1:B:247:ALA:HA	1:B:250:PHE:CE1	2.45	0.52
1:B:344:ASN:OD1	1:B:371:ARG:NH2	2.41	0.52
1:A:90:ASP:O	1:A:94:LEU:HG	2.10	0.52
1:B:293:ASP:HA	1:B:303:TRP:CH2	2.45	0.51
1:B:113:VAL:O	1:B:117:VAL:HG23	2.09	0.51
1:A:300:TRP:CZ2	1:A:326:ARG:NH2	2.78	0.51
1:B:429:ASN:N	1:B:429:ASN:ND2	2.57	0.51
1:B:160:ASN:ND2	1:B:261:LYS:HZ2	2.10	0.50
1:B:95:GLU:HG3	5:B:566:HOH:O	2.10	0.50
1:B:346:ILE:HG12	1:B:351:GLU:HB3	1.94	0.50
1:A:191:LEU:O	1:A:195:ILE:HG13	2.11	0.50
1:B:164:MET:CG	1:B:245:VAL:HG22	2.41	0.50
1:A:295:PHE:HB2	1:A:303:TRP:NE1	2.27	0.50
1:B:250:PHE:HB3	1:B:260:PHE:CD2	2.46	0.50
1:B:111:LEU:HD22	1:B:344:ASN:HA	1.94	0.50
1:B:284:ARG:HG2	5:B:519:HOH:O	2.12	0.49
1:A:370:HIS:CD2	1:A:370:HIS:H	2.29	0.49
1:A:9:GLU:HG3	1:A:61:VAL:HG22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLN:HA	1:A:337:ASN:HD21	1.76	0.49
1:A:142:LEU:HD22	1:A:142:LEU:N	2.27	0.49
1:A:40:THR:HG22	1:A:371:ARG:NH2	2.26	0.48
1:B:131:ARG:HG3	1:B:131:ARG:NH2	2.28	0.48
1:A:268:ARG:HG3	1:A:268:ARG:NH2	2.27	0.48
1:A:149:PHE:O	1:A:168:MET:HA	2.14	0.48
1:B:50:ASP:HA	1:B:63:LYS:HD2	1.96	0.48
1:B:149:PHE:O	1:B:168:MET:HA	2.13	0.48
1:B:47:GLU:HB3	5:B:493:HOH:O	2.13	0.48
1:B:393:LYS:O	1:B:393:LYS:HG3	2.14	0.48
1:A:314:ILE:H	1:A:337:ASN:ND2	2.11	0.48
1:A:178:ARG:HD2	5:A:643:HOH:O	2.15	0.47
1:B:160:ASN:ND2	1:B:261:LYS:NZ	2.62	0.47
1:B:43:TYR:HB2	1:B:321:VAL:HG21	1.97	0.47
1:A:164:MET:H	1:A:219:ASN:HD21	1.61	0.47
1:B:131:ARG:NE	1:B:142:LEU:HD11	2.27	0.47
1:B:370:HIS:O	1:B:371:ARG:HD2	2.14	0.47
1:B:43:TYR:HA	5:B:492:HOH:O	2.15	0.46
1:A:121:GLY:O	1:A:125:ARG:HG3	2.16	0.46
1:A:277:ALA:HB2	5:A:548:HOH:O	2.15	0.46
1:B:255:LYS:HB3	1:B:269:TYR:HB3	1.97	0.46
1:B:396:ALA:HB1	1:B:397:PRO:HD2	1.97	0.46
1:A:82:SER:HB3	1:A:84:VAL:HG22	1.98	0.46
1:B:150:ASN:O	1:B:396:ALA:HB2	2.16	0.46
1:A:43:TYR:HD1	5:A:514:HOH:O	1.99	0.46
1:A:165:GLN:HG2	1:A:166:GLU:CG	2.46	0.46
1:B:48:LEU:HD12	5:B:553:HOH:O	2.16	0.46
1:A:428:ARG:HB2	5:A:606:HOH:O	2.14	0.45
1:B:37:GLY:HA2	1:B:371:ARG:HB3	1.98	0.45
1:B:44:GLU:CB	1:B:345:GLN:HG2	2.46	0.45
1:B:384:VAL:HG21	1:B:392:ILE:HB	1.98	0.45
1:B:294:PRO:HD2	1:B:303:TRP:CH2	2.51	0.45
1:B:183:LEU:HD23	1:B:183:LEU:N	2.32	0.45
1:B:303:TRP:CE3	1:B:319:LEU:HD22	2.52	0.45
1:A:401:GLU:CG	1:A:402:ARG:NE	2.80	0.45
1:B:119:LYS:HD3	5:B:601:HOH:O	2.16	0.45
1:B:418:ASP:C	1:B:420:ALA:H	2.20	0.45
1:B:276:GLY:O	1:B:280:GLN:HG2	2.17	0.44
1:A:300:TRP:HZ3	1:A:330:ALA:HA	1.83	0.44
1:A:299:ASP:O	1:A:299:ASP:OD1	2.34	0.44
1:B:37:GLY:HA3	1:B:371:ARG:CZ	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LYS:O	1:A:162:LEU:C	2.56	0.44
1:B:166:GLU:HB2	1:B:244:ASP:HB3	1.99	0.44
1:A:370:HIS:ND1	1:A:402:ARG:NH1	2.63	0.44
1:A:366:VAL:O	1:A:389:THR:HB	2.18	0.44
1:B:129:LEU:HB3	1:B:382:ASP:OD2	2.18	0.44
1:B:164:MET:HG3	1:B:245:VAL:HG13	2.00	0.44
1:A:400:SER:CB	1:B:401:GLU:HB3	2.48	0.44
1:A:314:ILE:O	1:A:336:CYS:HB2	2.18	0.43
1:B:43:TYR:HD1	5:B:586:HOH:O	2.01	0.43
1:B:295:PHE:HB2	1:B:303:TRP:CD1	2.53	0.43
1:A:401:GLU:HG2	1:A:402:ARG:NE	2.33	0.43
1:B:370:HIS:CG	1:B:394:THR:HA	2.54	0.43
1:A:39:SER:HA	1:A:249:GLU:OE1	2.17	0.43
1:A:23:LEU:C	1:A:23:LEU:HD23	2.38	0.43
1:A:108:ASN:OD1	1:A:108:ASN:N	2.52	0.43
1:B:84:VAL:CG1	1:B:124:GLU:HG2	2.47	0.42
1:A:134:ALA:HB2	1:A:142:LEU:HD11	2.01	0.42
1:A:413:GLU:HG3	1:A:420:ALA:HB1	2.00	0.42
1:B:429:ASN:O	1:B:432:VAL:HG22	2.19	0.42
1:A:278:LEU:HG	1:A:282:PHE:CZ	2.55	0.42
1:B:187:VAL:HG21	1:B:239:ILE:CD1	2.49	0.42
1:B:152:ILE:CD1	1:B:226:VAL:HG23	2.49	0.42
1:A:178:ARG:HB2	5:A:643:HOH:O	2.18	0.42
1:A:183:LEU:O	1:A:187:VAL:HG23	2.19	0.42
1:B:403:LEU:HD13	1:B:403:LEU:HA	1.80	0.42
1:A:73:ALA:O	1:A:77:ILE:HG13	2.19	0.42
1:A:367:MET:SD	1:A:393:LYS:HG2	2.59	0.42
1:B:45:ALA:HB1	1:B:107:ALA:HB2	2.01	0.42
1:B:262:SER:O	1:B:263:PRO:C	2.58	0.42
1:A:300:TRP:HZ2	1:A:326:ARG:HH21	1.67	0.41
1:B:265:ASP:O	1:B:267:SER:N	2.53	0.41
1:A:396:ALA:C	1:A:398:CYS:H	2.23	0.41
1:B:42:ILE:HG12	1:B:297:GLN:OE1	2.21	0.41
1:A:251:TYR:OH	1:A:254:GLY:HA2	2.20	0.41
1:B:143:ILE:HD12	1:B:143:ILE:C	2.41	0.41
1:B:394:THR:O	1:B:402:ARG:HB3	2.21	0.41
1:A:303:TRP:CE3	1:A:319:LEU:HD22	2.56	0.41
1:A:370:HIS:CG	1:A:394:THR:HA	2.56	0.41
1:B:416:LEU:O	1:B:419:GLU:HG3	2.21	0.41
1:A:256:TYR:CD2	1:A:275:LEU:HD22	2.56	0.41
1:A:294:PRO:HD2	1:A:303:TRP:CH2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ILE:HG23	1:B:347:GLY:N	2.35	0.41
1:A:271:THR:H	1:A:274:GLN:NE2	2.19	0.41
1:A:165:GLN:NE2	1:A:166:GLU:OE2	2.54	0.40
1:A:178:ARG:HH21	1:A:178:ARG:HG2	1.86	0.40
1:A:286:TYR:HB3	1:A:287:PRO:HD2	2.03	0.40
1:B:323:ASN:HD21	1:B:325:LYS:HE3	1.86	0.40
1:A:131:ARG:NH1	1:A:142:LEU:HD21	2.35	0.40
1:B:160:ASN:HD22	1:B:160:ASN:C	2.25	0.40
1:B:38:ALA:HB2	1:B:372:SER:OG	2.21	0.40
1:B:21:VAL:O	1:B:31:ARG:HA	2.21	0.40
1:B:323:ASN:O	1:B:327:ILE:HG13	2.21	0.40
1:A:183:LEU:HB3	1:A:239:ILE:HD11	2.02	0.40
1:A:359:ALA:O	1:A:364:TRP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/439 (98%)	401 (93%)	29 (7%)	1 (0%)	47	38
1	B	430/439 (98%)	398 (93%)	29 (7%)	3 (1%)	22	11
All	All	861/878 (98%)	799 (93%)	58 (7%)	4 (0%)	29	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	PRO
1	B	266	PRO
1	B	419	GLU
1	A	399	ARG

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	335/356 (94%)	329 (98%)	6 (2%)	59	53
1	B	339/356 (95%)	326 (96%)	13 (4%)	33	22
All	All	674/712 (95%)	655 (97%)	19 (3%)	43	34

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	MET
1	A	252	ARG
1	A	337	ASN
1	A	348	SER
1	A	370	HIS
1	A	393	LYS
1	B	8	ARG
1	B	101	ASN
1	B	150	ASN
1	B	153	ASN
1	B	160	ASN
1	B	164	MET
1	B	183	LEU
1	B	263	PRO
1	B	264	THR
1	B	273	ASP
1	B	318	ASP
1	B	370	HIS
1	B	429	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	135	GLN
1	A	150	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	189	HIS
1	A	215	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	150	ASN
1	B	153	ASN
1	B	160	ASN
1	B	323	ASN
1	B	345	GLN
1	B	429	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	460	-	7,7,7	0.82	0	9,9,9	2.03	4 (44%)
3	PO4	A	442	2	4,4,4	1.71	1 (25%)	6,6,6	0.42	0
3	PO4	B	442	-	4,4,4	1.65	0	6,6,6	0.42	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	460	-	-	3/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	442	PO4	P-O2	-2.06	1.48	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	460	TRS	O1-C1-C	3.71	122.74	111.00
4	A	460	TRS	C2-C-N	3.47	118.35	107.98
4	A	460	TRS	O2-C2-C	2.16	117.86	111.00
4	A	460	TRS	C1-C-N	-2.11	101.68	107.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	460	TRS	C3-C-C2-O2
4	A	460	TRS	C1-C-C2-O2
4	A	460	TRS	N-C-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	442	PO4	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	433/439 (98%)	0.66	37 (8%)	10	12	17, 33, 60, 71	0
1	B	432/439 (98%)	0.40	22 (5%)	28	31	17, 31, 53, 74	0
All	All	865/878 (98%)	0.53	59 (6%)	17	19	17, 32, 57, 74	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	PHE	5.8
1	B	263	PRO	4.6
1	A	266	PRO	4.4
1	A	264	THR	4.4
1	A	217	LEU	4.1
1	B	159	GLY	4.0
1	A	275	LEU	3.8
1	B	264	THR	3.7
1	A	380	ILE	3.6
1	A	278	LEU	3.5
1	A	406	TYR	3.5
1	B	142	LEU	3.5
1	B	46	LEU	3.5
1	B	41	GLY	3.4
1	B	38	ALA	3.2
1	A	263	PRO	3.2
1	A	251	TYR	3.2
1	A	418	ASP	3.2
1	A	404	ALA	3.0
1	B	43	TYR	3.0
1	A	403	LEU	2.9
1	A	269	TYR	2.9
1	B	40	THR	2.8
1	B	141	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	271	THR	2.8
1	A	42	ILE	2.7
1	A	256	TYR	2.7
1	A	163	ALA	2.7
1	B	262	SER	2.7
1	A	265	ASP	2.6
1	A	270	ILE	2.6
1	B	36	SER	2.6
1	A	253	ASP	2.5
1	A	301	ALA	2.5
1	B	158	ALA	2.5
1	A	258	LEU	2.5
1	B	39	SER	2.4
1	A	302	ALA	2.4
1	B	98	GLY	2.4
1	A	400	SER	2.3
1	A	420	ALA	2.3
1	A	325	LYS	2.3
1	B	429	ASN	2.3
1	B	157	HIS	2.3
1	B	375	THR	2.3
1	B	431	SER	2.3
1	B	404	ALA	2.2
1	A	125	ARG	2.2
1	A	237	GLU	2.2
1	A	383	LEU	2.1
1	A	262	SER	2.1
1	A	254	GLY	2.1
1	A	306	PHE	2.1
1	B	418	ASP	2.1
1	A	379	PHE	2.1
1	A	384	VAL	2.1
1	B	400	SER	2.1
1	A	34	VAL	2.0
1	A	272	GLY	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 monosaccharides 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
4	TRS	A	460	8/8	0.76	0.23	55,58,60,60	0
3	PO4	B	442	5/5	0.88	0.17	46,46,48,48	0
2	MG	A	441	1/1	0.90	0.07	38,38,38,38	0
2	MG	B	440	1/1	0.92	0.10	29,29,29,29	0
2	MG	A	440	1/1	0.94	0.07	39,39,39,39	0
3	PO4	A	442	5/5	0.98	0.12	32,32,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.