Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:27 PM BST

PDB ID	:	7BR2
Title	:	BT4096 a gut microbial diltiazem-metabolizing enzyme
Authors	:	Ko, T.-P.; Chen, C.-C.; Guo, R.-T.
Deposited on	:	2020-03-26
Resolution	:	2.33 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 following versions of software and data (see references ①) were used in the production of this report:

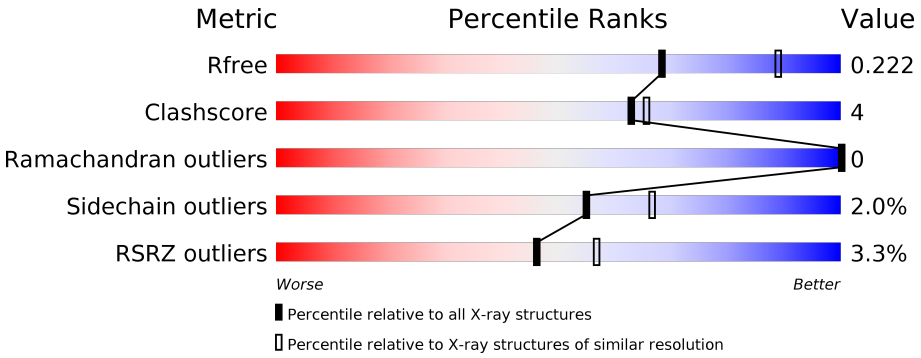
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 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	450	4% 85% 14%
1	B	450	4% 88% 10%
1	C	450	3% 87% 10%
1	D	450	3% 88% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15461 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 Lipolytic enzyme, G-D-S-L family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3615	2297	620	676	22			
1	B	443	Total	C	N	O	S	0	0	0
			3602	2290	617	673	22			
1	C	442	Total	C	N	O	S	0	0	0
			3597	2287	616	672	22			
1	D	446	Total	C	N	O	S	0	0	0
			3615	2297	620	676	22			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q8A0C5
A	-8	ALA	-	expression tag	UNP Q8A0C5
A	-7	GLY	-	expression tag	UNP Q8A0C5
A	-6	ALA	-	expression tag	UNP Q8A0C5
A	-5	GLY	-	expression tag	UNP Q8A0C5
A	-4	ALA	-	expression tag	UNP Q8A0C5
A	-3	GLY	-	expression tag	UNP Q8A0C5
A	-2	ALA	-	expression tag	UNP Q8A0C5
A	-1	GLY	-	expression tag	UNP Q8A0C5
A	0	ALA	-	expression tag	UNP Q8A0C5
B	-9	GLY	-	expression tag	UNP Q8A0C5
B	-8	ALA	-	expression tag	UNP Q8A0C5
B	-7	GLY	-	expression tag	UNP Q8A0C5
B	-6	ALA	-	expression tag	UNP Q8A0C5
B	-5	GLY	-	expression tag	UNP Q8A0C5
B	-4	ALA	-	expression tag	UNP Q8A0C5
B	-3	GLY	-	expression tag	UNP Q8A0C5
B	-2	ALA	-	expression tag	UNP Q8A0C5
B	-1	GLY	-	expression tag	UNP Q8A0C5
B	0	ALA	-	expression tag	UNP Q8A0C5
C	-9	GLY	-	expression tag	UNP Q8A0C5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	ALA	-	expression tag	UNP Q8A0C5
C	-7	GLY	-	expression tag	UNP Q8A0C5
C	-6	ALA	-	expression tag	UNP Q8A0C5
C	-5	GLY	-	expression tag	UNP Q8A0C5
C	-4	ALA	-	expression tag	UNP Q8A0C5
C	-3	GLY	-	expression tag	UNP Q8A0C5
C	-2	ALA	-	expression tag	UNP Q8A0C5
C	-1	GLY	-	expression tag	UNP Q8A0C5
C	0	ALA	-	expression tag	UNP Q8A0C5
D	-9	GLY	-	expression tag	UNP Q8A0C5
D	-8	ALA	-	expression tag	UNP Q8A0C5
D	-7	GLY	-	expression tag	UNP Q8A0C5
D	-6	ALA	-	expression tag	UNP Q8A0C5
D	-5	GLY	-	expression tag	UNP Q8A0C5
D	-4	ALA	-	expression tag	UNP Q8A0C5
D	-3	GLY	-	expression tag	UNP Q8A0C5
D	-2	ALA	-	expression tag	UNP Q8A0C5
D	-1	GLY	-	expression tag	UNP Q8A0C5
D	0	ALA	-	expression tag	UNP Q8A0C5

- Molecule 2 is water.

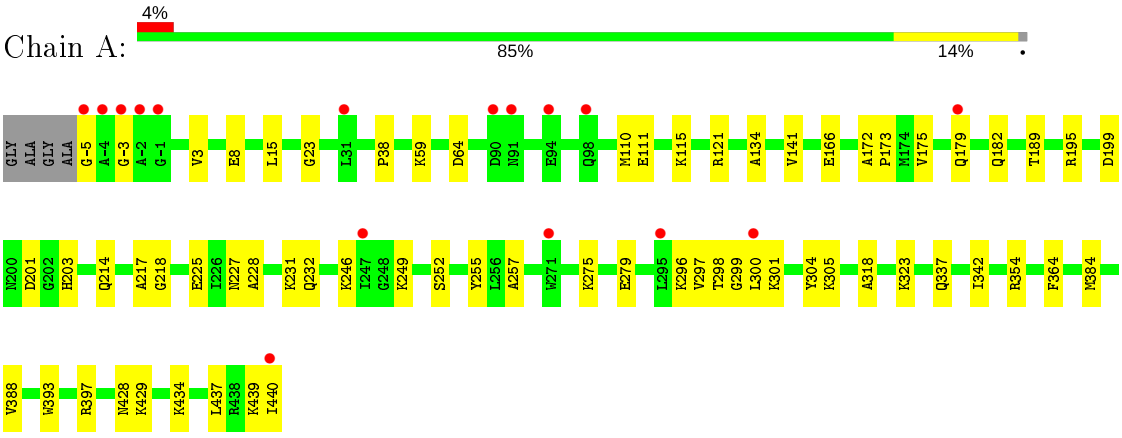
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	258	Total	O	0	0
			258	258		
2	B	238	Total	O	0	0
			238	238		
2	C	276	Total	O	0	0
			276	276		
2	D	260	Total	O	0	0
			260	260		

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.

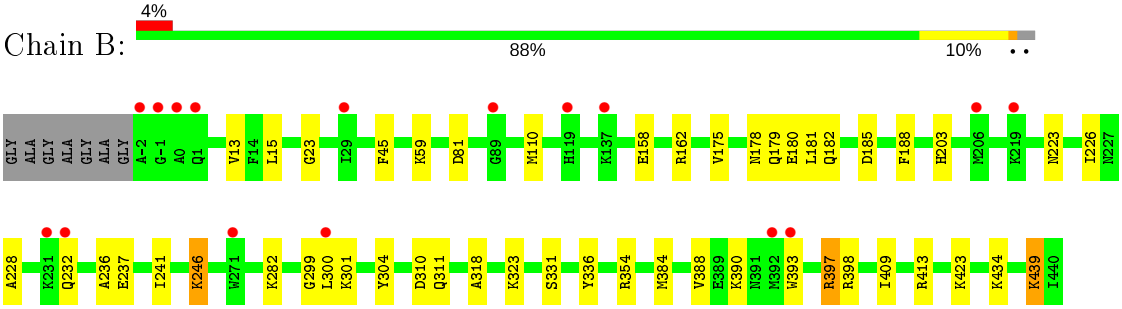
- Molecule 1: Lipolytic enzyme, G-D-S-L family

Chain A:



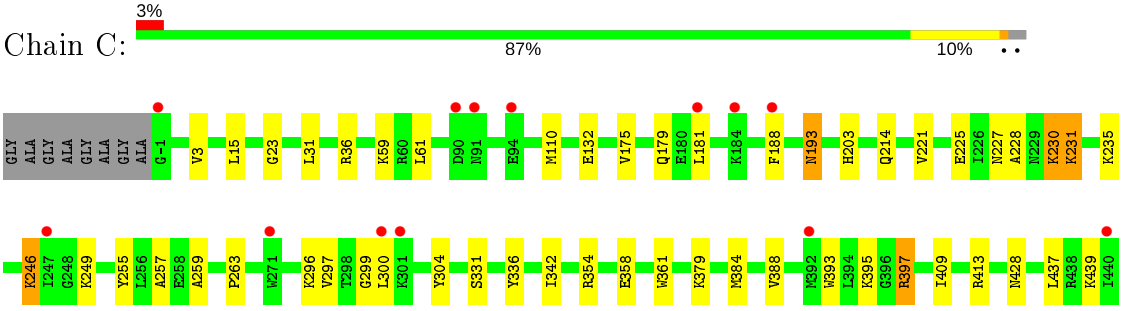
- Molecule 1: Lipolytic enzyme, G-D-S-L family

Chain B:



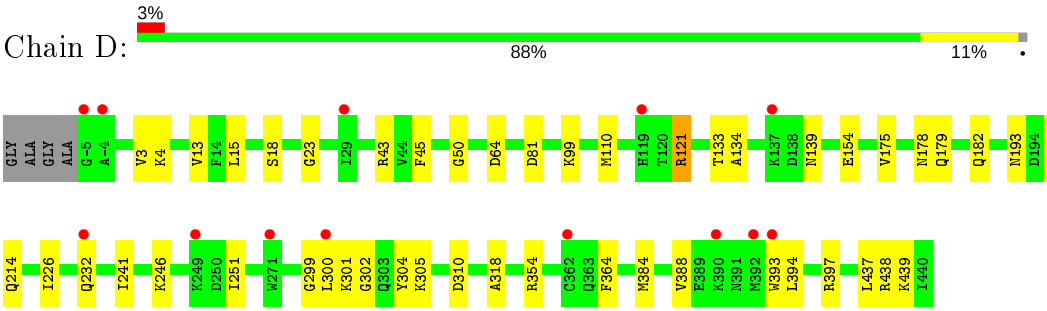
- Molecule 1: Lipolytic enzyme, G-D-S-L family

Chain C:



- Molecule 1: Lipolytic enzyme, G-D-S-L family

Chain D:


3%
88%
11%
GLY ALA GLY ALA G-5 A-4 V3 K4 V13 F14 L15 S18 G23 I29 R43 V44 F45 G50 D64 D81 K99 M110 H119 T120 R121 T133 A134 K137 D138 N139 E154 V175 N178 Q179 Q182 N193 D194 R195 H203
Q214 I226 Q232 I241 K246 K249 D250 I251 W271 G299 L300 K301 G302 Q303 Y304 K305 D310 A318 R354 C362 Q363 F364 M384 V388 E389 K390 N391 M392 W393 L394 R397 L437 R438 K439 I440

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.69Å 133.80Å 182.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.94 – 2.33 24.94 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.94-2.33) 95.1 (24.94-2.33)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 2.33Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.182 , 0.222 0.182 , 0.222	Depositor DCC
R_{free} test set	2000 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15461	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0261e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0/3691	0.58	1/4962 (0.0%)
1	B	0.41	0/3678	0.59	0/4945
1	C	0.41	0/3673	0.59	0/4938
1	D	0.42	0/3691	0.59	0/4962
All	All	0.41	0/14733	0.59	1/19807 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	300	LEU	CB-CG-CD1	-5.40	101.83	111.00

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	3615	0	3569	35	0
1	B	3602	0	3558	28	0
1	C	3597	0	3553	30	0
1	D	3615	0	3569	32	0
2	A	258	0	0	1	0
2	B	238	0	0	8	0
2	C	276	0	0	2	0
2	D	260	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15461	0	14249	124	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 4.

All (124) 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:134:ALA:O	1:A:195:ARG:NH1	2.06	0.88
1:D:134:ALA:O	1:D:195:ARG:NH2	2.09	0.85
1:B:393:TRP:O	1:B:397:ARG:NH1	2.17	0.78
1:D:232:GLN:O	2:D:501:HOH:O	2.02	0.76
1:D:226:ILE:HD11	1:D:241:ILE:HG21	1.67	0.76
1:D:4:LYS:O	1:D:121:ARG:NH2	2.22	0.72
1:D:301:LYS:NZ	2:D:503:HOH:O	2.22	0.71
1:C:15:LEU:HD21	1:C:110:MET:HE1	1.74	0.70
1:D:15:LEU:HD21	1:D:110:MET:HE1	1.75	0.69
1:C:388:VAL:HB	1:C:395:LYS:HG3	1.73	0.69
1:C:228:ALA:HB3	1:C:299:GLY:HA3	1.74	0.68
1:D:154:GLU:OE1	2:D:502:HOH:O	2.13	0.67
1:B:15:LEU:HD21	1:B:110:MET:HE1	1.77	0.66
1:B:226:ILE:HD11	1:B:241:ILE:HG21	1.79	0.63
1:C:249:LYS:HD2	1:C:300:LEU:HD21	1.80	0.63
1:A:8:GLU:OE2	1:D:305:LYS:NZ	2.31	0.62
1:D:23:GLY:HA3	1:D:203:HIS:CE1	2.35	0.61
1:A:304:TYR:CE2	1:A:439:LYS:HB2	2.36	0.60
1:B:384:MET:O	1:B:388:VAL:HG13	2.01	0.60
1:C:23:GLY:HA3	1:C:203:HIS:CE1	2.37	0.59
1:D:301:LYS:HA	1:D:318:ALA:HB3	1.85	0.58
1:A:23:GLY:HA3	1:A:203:HIS:CE1	2.39	0.58
1:A:301:LYS:HA	1:A:318:ALA:HB3	1.84	0.58
1:B:181:LEU:HD12	1:B:188:PHE:CZ	2.39	0.58
1:D:299:GLY:O	1:D:301:LYS:HD3	2.04	0.58
1:A:305:LYS:HB2	1:A:440:ILE:HD11	1.86	0.57
1:B:232:GLN:O	2:B:501:HOH:O	2.17	0.57
1:B:180:GLU:OE2	2:B:502:HOH:O	2.17	0.57
1:A:-3:GLY:HA3	1:A:217:ALA:HB3	1.86	0.57
1:C:193:ASN:ND2	2:C:501:HOH:O	2.21	0.54
1:C:384:MET:O	1:C:388:VAL:HG13	2.08	0.54
1:C:175:VAL:O	1:C:179:GLN:HG2	2.08	0.53
1:B:304:TYR:CE2	1:B:439:LYS:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ARG:NH1	2:D:508:HOH:O	2.32	0.52
1:B:300:LEU:O	2:B:503:HOH:O	2.19	0.52
1:A:384:MET:O	1:A:388:VAL:HG13	2.09	0.52
1:D:301:LYS:HA	1:D:318:ALA:CB	2.40	0.52
1:B:301:LYS:HA	1:B:318:ALA:CB	2.40	0.52
1:D:302:GLY:HA3	1:D:439:LYS:NZ	2.24	0.51
1:B:23:GLY:HA3	1:B:203:HIS:CE1	2.46	0.51
1:D:300:LEU:HG	1:D:301:LYS:H	1.76	0.50
1:A:393:TRP:O	1:A:397:ARG:HD2	2.11	0.50
1:D:175:VAL:O	1:D:179:GLN:HG2	2.12	0.50
1:A:227:ASN:HA	1:A:298:THR:O	2.11	0.50
1:C:249:LYS:HD2	1:C:300:LEU:CD2	2.40	0.50
1:C:361:TRP:CZ2	1:C:393:TRP:HD1	2.29	0.50
1:A:301:LYS:HA	1:A:318:ALA:CB	2.42	0.49
1:B:282:LYS:NZ	2:B:517:HOH:O	2.45	0.49
1:D:43:ARG:HG2	1:D:45:PHE:CE1	2.48	0.49
1:A:64:ASP:HB2	1:A:364:PHE:CE2	2.48	0.49
1:A:111:GLU:O	1:A:115:LYS:HG3	2.13	0.48
1:C:379:LYS:HG2	2:C:677:HOH:O	2.13	0.48
1:B:175:VAL:O	1:B:179:GLN:HG2	2.13	0.48
1:C:59:LYS:HE3	1:C:59:LYS:HB2	1.51	0.47
1:B:59:LYS:HB2	1:B:59:LYS:HE3	1.62	0.47
1:B:182:GLN:HA	1:B:185:ASP:O	2.14	0.47
1:B:331:SER:HA	1:B:336:TYR:CD2	2.49	0.47
1:B:228:ALA:HB3	1:B:299:GLY:HA3	1.95	0.47
1:D:384:MET:O	1:D:388:VAL:HG13	2.14	0.47
1:D:3:VAL:O	1:D:214:GLN:HA	2.15	0.47
1:A:134:ALA:HB2	1:A:182:GLN:NE2	2.30	0.47
1:A:175:VAL:O	1:A:179:GLN:HG2	2.15	0.46
1:A:201:ASP:HB3	1:A:279:GLU:HB3	1.98	0.46
1:C:181:LEU:HB2	1:C:188:PHE:CE2	2.50	0.46
1:C:361:TRP:CH2	1:C:393:TRP:HD1	2.33	0.46
1:A:225:GLU:HA	1:A:296:LYS:O	2.15	0.46
1:A:228:ALA:HB3	1:A:299:GLY:HA3	1.97	0.46
1:D:178:ASN:O	1:D:182:GLN:HB2	2.16	0.46
1:D:64:ASP:HB2	1:D:364:PHE:CE2	2.50	0.46
1:A:252:SER:HB2	1:A:434:LYS:HE2	1.98	0.46
1:C:255:TYR:CZ	1:C:257:ALA:HB2	2.51	0.46
1:C:304:TYR:CE2	1:C:439:LYS:HB3	2.51	0.46
1:D:139:ASN:OD1	1:D:195:ARG:HD2	2.16	0.46
1:D:438:ARG:NH1	2:D:506:HOH:O	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PRO:O	1:A:429:LYS:NZ	2.49	0.45
1:A:297:VAL:HG21	1:A:437:LEU:HD11	1.98	0.45
1:B:311:GLN:HB2	2:B:700:HOH:O	2.16	0.45
1:D:18:SER:HB3	1:D:50:GLY:HA2	1.97	0.45
1:A:-5:GLY:HA3	1:A:218:GLY:HA2	1.97	0.45
1:C:297:VAL:HG21	1:C:437:LEU:HD11	1.98	0.45
1:B:301:LYS:HE2	2:B:610:HOH:O	2.16	0.44
1:B:311:GLN:HG2	2:B:534:HOH:O	2.17	0.44
1:A:141:VAL:HG22	1:A:195:ARG:CZ	2.47	0.44
1:C:388:VAL:HB	1:C:395:LYS:CG	2.44	0.44
1:D:13:VAL:HG22	1:D:45:PHE:HB2	2.00	0.44
1:C:31:LEU:HD21	1:C:263:PRO:HG2	1.99	0.43
1:D:301:LYS:HB3	2:D:599:HOH:O	2.16	0.43
1:B:178:ASN:O	1:B:182:GLN:HB2	2.19	0.43
1:C:358:GLU:OE1	1:C:397:ARG:NE	2.51	0.43
1:D:133:THR:HG21	1:D:179:GLN:HE22	1.84	0.43
1:C:225:GLU:HG3	1:C:296:LYS:HD2	2.00	0.43
1:C:61:LEU:HA	1:C:61:LEU:HD23	1.87	0.43
1:C:231:LYS:HD3	1:C:246:LYS:HB2	1.99	0.42
1:A:255:TYR:CZ	1:A:257:ALA:HB2	2.54	0.42
1:C:409:ILE:O	1:C:413:ARG:HG2	2.20	0.42
1:A:15:LEU:HD21	1:A:110:MET:HE1	2.01	0.42
1:A:189:THR:O	1:A:275:LYS:NZ	2.53	0.42
1:B:158:GLU:O	1:B:162:ARG:HG3	2.20	0.42
1:C:227:ASN:HB3	1:C:230:LYS:HB2	2.02	0.42
1:C:36:ARG:HA	1:C:259:ALA:HB1	2.01	0.42
1:A:337:GLN:NE2	2:A:521:HOH:O	2.52	0.42
1:A:121:ARG:NH1	1:A:166:GLU:OE2	2.44	0.41
1:A:231:LYS:HE2	1:A:231:LYS:HB3	1.59	0.41
1:A:59:LYS:HE3	1:A:59:LYS:HB2	1.58	0.41
1:B:236:ALA:O	2:B:504:HOH:O	2.22	0.41
1:D:251:ILE:CG2	1:D:437:LEU:HB2	2.50	0.41
1:A:342:ILE:HD11	1:A:428:ASN:HA	2.01	0.41
1:D:251:ILE:HG22	1:D:437:LEU:HB2	2.02	0.41
1:C:331:SER:HA	1:C:336:TYR:CD2	2.56	0.41
1:B:223:ASN:HB3	1:B:237:GLU:HB2	2.03	0.41
1:B:423:LYS:HA	1:B:423:LYS:HD3	1.82	0.41
1:C:36:ARG:CZ	1:C:221:VAL:HG22	2.51	0.41
1:D:304:TYR:CZ	1:D:439:LYS:HD2	2.55	0.41
1:D:300:LEU:HG	1:D:301:LYS:N	2.36	0.40
1:A:172:ALA:HB3	1:A:173:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:VAL:O	1:C:214:GLN:HA	2.21	0.40
1:A:199:ASP:HB3	1:A:201:ASP:OD1	2.20	0.40
1:B:409:ILE:O	1:B:413:ARG:HG2	2.21	0.40
1:A:297:VAL:HG21	1:A:437:LEU:CD1	2.52	0.40
1:A:3:VAL:O	1:A:214:GLN:HA	2.21	0.40
1:B:13:VAL:HG22	1:B:45:PHE:HB2	2.04	0.40
1:B:246:LYS:HB3	1:B:246:LYS:HE2	1.80	0.40
1:C:342:ILE:HD11	1:C:428:ASN:HA	2.03	0.40
1:D:393:TRP:CZ2	1:D:397:ARG:NH1	2.90	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	444/450 (99%)	432 (97%)	12 (3%)	0	100	100
1	B	441/450 (98%)	429 (97%)	12 (3%)	0	100	100
1	C	440/450 (98%)	429 (98%)	11 (2%)	0	100	100
1	D	444/450 (99%)	432 (97%)	12 (3%)	0	100	100
All	All	1769/1800 (98%)	1722 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	381/381 (100%)	376 (99%)	5 (1%)	69 79
1	B	381/381 (100%)	371 (97%)	10 (3%)	46 56
1	C	381/381 (100%)	373 (98%)	8 (2%)	53 65
1	D	381/381 (100%)	373 (98%)	8 (2%)	53 65
All	All	1524/1524 (100%)	1493 (98%)	31 (2%)	55 66

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	GLN
1	A	246	LYS
1	A	249	LYS
1	A	323	LYS
1	A	354	ARG
1	B	81	ASP
1	B	246	LYS
1	B	310	ASP
1	B	323	LYS
1	B	354	ARG
1	B	390	LYS
1	B	397	ARG
1	B	398	ARG
1	B	434	LYS
1	B	439	LYS
1	C	132	GLU
1	C	193	ASN
1	C	230	LYS
1	C	231	LYS
1	C	235	LYS
1	C	246	LYS
1	C	354	ARG
1	C	397	ARG
1	D	81	ASP
1	D	99	LYS
1	D	121	ARG
1	D	193	ASN
1	D	246	LYS
1	D	310	ASP
1	D	354	ARG
1	D	394	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	ASN
1	B	337	GLN
1	B	344	HIS
1	C	98	GLN
1	C	243	ASN
1	D	69	ASN
1	D	179	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	446/450 (99%)	-0.08	16 (3%)	42	53	24, 38, 64, 81	0
1	B	443/450 (98%)	-0.09	16 (3%)	42	53	24, 37, 61, 101	0
1	C	442/450 (98%)	-0.22	13 (2%)	51	61	24, 36, 69, 87	0
1	D	446/450 (99%)	-0.16	13 (2%)	51	61	22, 36, 62, 104	0
All	All	1777/1800 (98%)	-0.14	58 (3%)	46	57	22, 37, 64, 104	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-4	ALA	7.3
1	B	-2	ALA	6.7
1	A	-2	ALA	6.7
1	B	-1	GLY	5.8
1	C	300	LEU	5.2
1	A	271	TRP	5.2
1	C	271	TRP	4.9
1	A	-5	GLY	4.7
1	A	-3	GLY	4.7
1	A	300	LEU	4.6
1	D	300	LEU	4.5
1	D	271	TRP	4.3
1	B	271	TRP	4.1
1	B	300	LEU	4.0
1	B	231	LYS	3.6
1	C	184	LYS	3.6
1	B	0	ALA	3.5
1	D	137	LYS	3.2
1	D	392	MET	3.2
1	D	-5	GLY	3.2
1	C	-1	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	393	TRP	3.1
1	B	137	LYS	3.0
1	D	232	GLN	2.9
1	C	247	ILE	2.8
1	C	440	ILE	2.8
1	A	90	ASP	2.7
1	B	392	MET	2.7
1	C	392	MET	2.7
1	D	249	LYS	2.7
1	A	-1	GLY	2.7
1	A	295	LEU	2.6
1	A	440	ILE	2.6
1	B	119	HIS	2.6
1	A	91	ASN	2.5
1	B	232	GLN	2.5
1	B	29	ILE	2.5
1	B	89	GLY	2.5
1	C	90	ASP	2.5
1	D	-4	ALA	2.4
1	D	362	CYS	2.4
1	A	98	GLN	2.3
1	D	390	LYS	2.3
1	C	94	GLU	2.3
1	A	94	GLU	2.3
1	D	119	HIS	2.3
1	A	31	LEU	2.2
1	C	188	PHE	2.1
1	C	301	LYS	2.1
1	B	206	MET	2.1
1	C	91	ASN	2.1
1	A	247	ILE	2.1
1	D	29	ILE	2.1
1	B	393	TRP	2.1
1	A	179	GLN	2.0
1	B	1	GLN	2.0
1	C	181	LEU	2.0
1	B	219	LYS	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

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.