Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2020 – 10:03 AM EDT

PDB ID	:	6X88
Title	:	PDE6 chicken GAF domain
Authors	:	Ke, H.
Deposited on	:	2020-06-01
Resolution	:	3.20 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 ⓘ) were used in the production of this report:

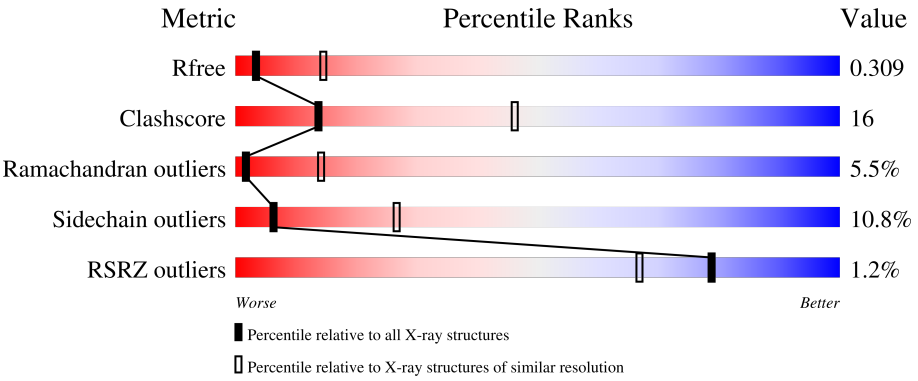
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	862	25% 15% · 56%
1	B	862	% 25% 16% · 56%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6151 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 Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha'.

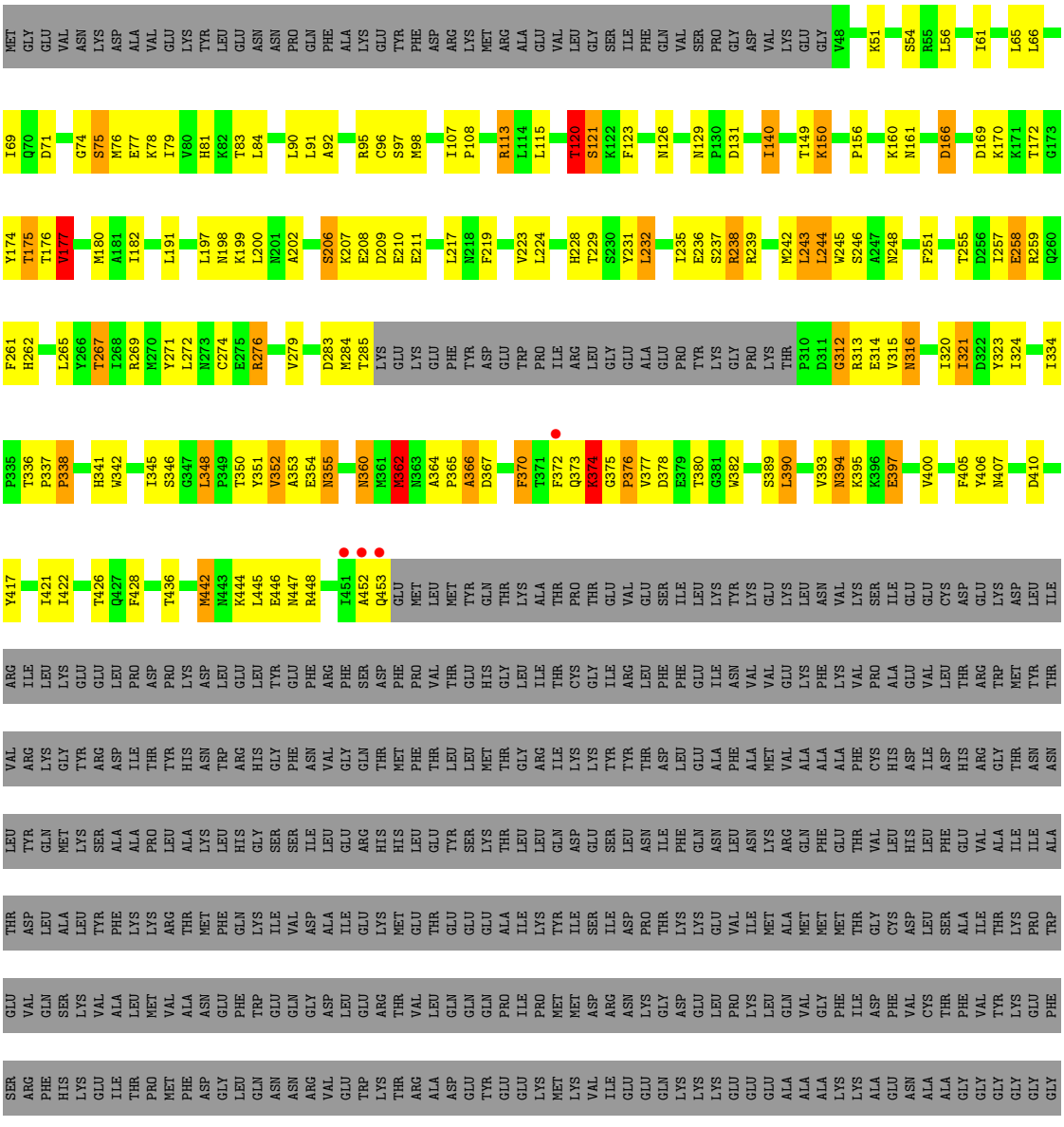
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3103	1987	514	584	18			
1	B	375	Total	C	N	O	S	0	0	0
			3048	1952	506	573	17			

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.

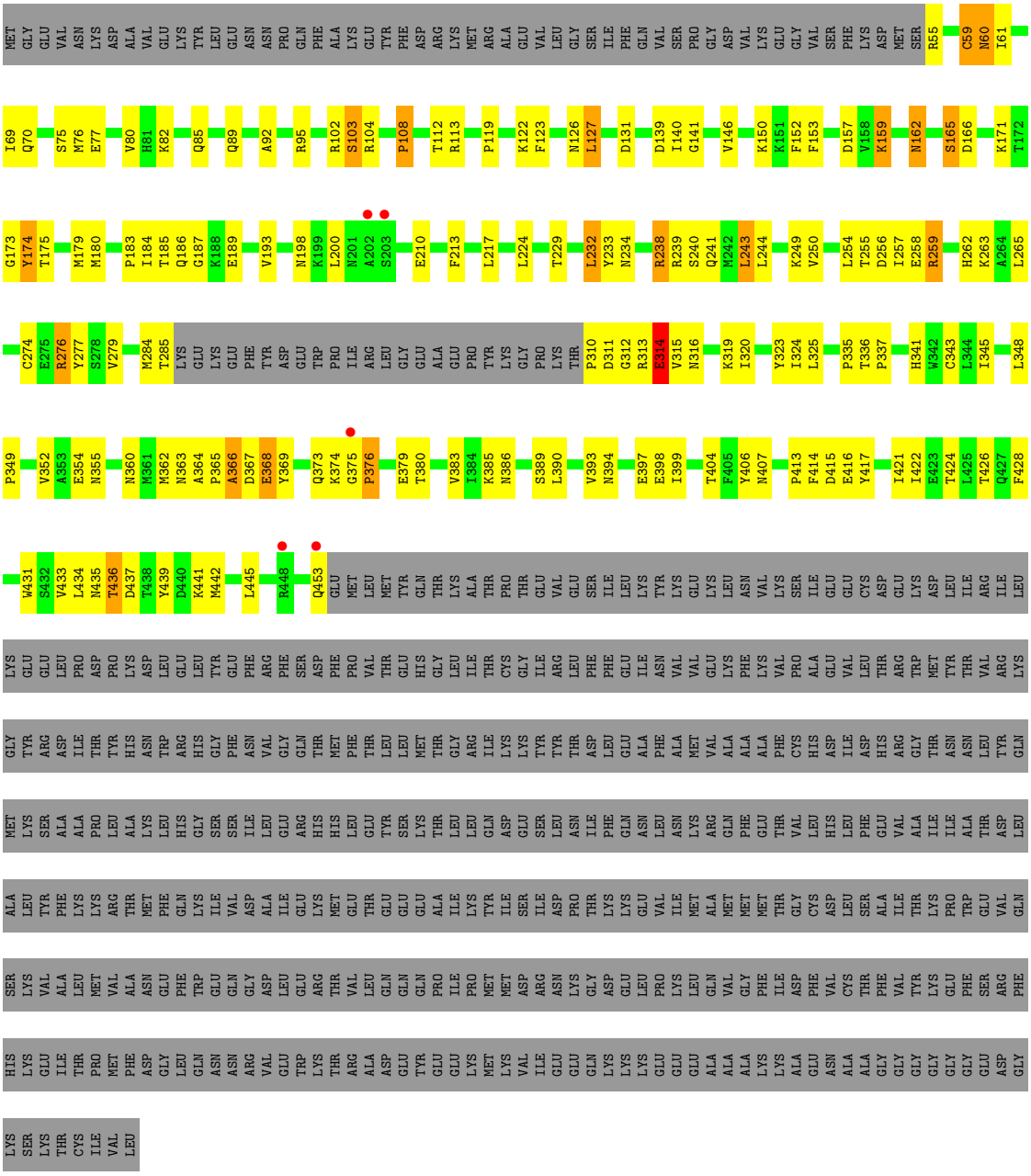
• Molecule 1: Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha'

Chain A: 25% 15% 56%



• Molecule 1: Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha'

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	148.50Å 148.50Å 93.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.98 – 3.20 43.15 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.0 (38.98-3.20) 89.0 (43.15-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10_2155, PHENIX 1.10_2155	Depositor
R, R_{free}	0.210 , 0.307 0.209 , 0.309	Depositor DCC
R_{free} test set	911 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	75.7	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6151	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

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	0.61	1/3169 (0.0%)	0.89	8/4285 (0.2%)
1	B	0.60	0/3113	0.88	3/4211 (0.1%)
All	All	0.60	1/6282 (0.0%)	0.89	11/8496 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	THR	C-O	7.82	1.38	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	285	THR	CA-C-O	19.20	160.43	120.10
1	A	453	GLN	CA-C-O	-16.70	85.03	120.10
1	B	453	GLN	CA-C-O	-16.17	86.13	120.10
1	A	285	THR	CA-C-O	6.72	134.21	120.10
1	A	276	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	362	MET	N-CA-C	-6.13	94.44	111.00
1	B	238	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	269	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	238	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	276	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	362	MET	CA-CB-CG	5.01	121.82	113.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	314	GLU	Peptide
1	A	410	ASP	Peptide
1	B	314	GLU	Peptide

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	3103	0	3079	114	0
1	B	3048	0	3025	86	0
All	All	6151	0	6104	195	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 (195) 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:95:ARG:NH2	1:A:174:TYR:O	2.11	0.83
1:A:390:LEU:HD21	1:A:422:ILE:HG22	1.60	0.83
1:A:276:ARG:CZ	1:A:324:ILE:HD13	2.16	0.76
1:A:376:PRO:CB	1:A:377:VAL:HA	2.17	0.74
1:A:336:THR:HG22	1:A:336:THR:O	1.93	0.69
1:B:256:ASP:OD1	1:B:259:ARG:HG3	1.95	0.65
1:A:265:LEU:HD13	1:A:279:VAL:HG21	1.77	0.64
1:A:276:ARG:HB2	1:A:406:TYR:HB2	1.78	0.64
1:A:346:SER:HA	1:A:370:PHE:O	1.99	0.62
1:B:77:GLU:OE2	1:B:113:ARG:NH1	2.29	0.61
1:B:389:SER:HB3	1:B:404:THR:HG23	1.82	0.61
1:A:182:ILE:HG21	1:A:217:LEU:HD13	1.82	0.61
1:B:265:LEU:HD11	1:B:279:VAL:HG21	1.81	0.60
1:A:394:ASN:HB3	1:A:397:GLU:H	1.65	0.60
1:A:98:MET:CE	1:A:224:LEU:HD11	2.32	0.60
1:A:238:ARG:NH1	1:A:271:TYR:O	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LEU:CD1	1:B:279:VAL:HG21	2.32	0.59
1:A:77:GLU:OE2	1:A:113:ARG:NH2	2.36	0.59
1:A:69:ILE:HD13	1:A:223:VAL:HG22	1.85	0.59
1:B:436:THR:HG22	1:B:437:ASP:N	2.18	0.58
1:A:350:THR:O	1:A:353:ALA:HB3	2.03	0.58
1:B:368:GLU:O	1:B:369:TYR:CG	2.58	0.57
1:A:284:MET:SD	1:A:400:VAL:HG22	2.45	0.57
1:B:173:GLY:O	1:B:175:THR:N	2.38	0.57
1:A:74:GLY:HA3	1:A:75:SER:CB	2.35	0.56
1:A:265:LEU:CD1	1:A:279:VAL:HG21	2.35	0.56
1:B:95:ARG:NH2	1:B:174:TYR:O	2.39	0.56
1:B:59:CYS:O	1:B:61:ILE:N	2.39	0.56
1:A:336:THR:O	1:A:336:THR:CG2	2.54	0.55
1:A:374:LYS:HB3	1:A:376:PRO:HB2	1.89	0.55
1:A:257:ILE:HG23	1:A:258:GLU:H	1.71	0.54
1:A:176:THR:O	1:A:177:VAL:HG13	2.08	0.54
1:B:239:ARG:HB2	1:B:421:ILE:HG22	1.90	0.54
1:B:312:GLY:O	1:B:314:GLU:N	2.34	0.54
1:B:352:VAL:O	1:B:355:ASN:O	2.26	0.54
1:A:393:VAL:O	1:A:394:ASN:O	2.26	0.53
1:A:81:HIS:HA	1:A:84:LEU:HD12	1.91	0.53
1:B:152:PHE:CD1	1:B:153:PHE:N	2.76	0.53
1:B:393:VAL:HG12	1:B:397:GLU:HA	1.90	0.53
1:B:428:PHE:O	1:B:428:PHE:CG	2.62	0.53
1:A:378:ASP:HB3	1:A:380:THR:N	2.24	0.53
1:A:376:PRO:HB3	1:A:377:VAL:HA	1.90	0.52
1:A:245:TRP:O	1:A:246:SER:C	2.44	0.52
1:B:150:LYS:HA	1:B:183:PRO:HG3	1.93	0.51
1:A:375:GLY:N	1:A:376:PRO:HD2	2.25	0.51
1:B:243:LEU:CD1	1:B:424:THR:HG22	2.41	0.51
1:A:312:GLY:HA2	1:A:354:GLU:HB3	1.93	0.51
1:B:243:LEU:HD11	1:B:424:THR:HG22	1.91	0.51
1:A:257:ILE:HG23	1:A:258:GLU:N	2.25	0.51
1:A:258:GLU:HG2	1:A:259:ARG:N	2.24	0.51
1:A:352:VAL:O	1:A:355:ASN:O	2.27	0.51
1:A:74:GLY:HA3	1:A:75:SER:HB2	1.91	0.51
1:A:374:LYS:HB3	1:A:376:PRO:CB	2.41	0.51
1:B:239:ARG:HG3	1:B:424:THR:HG21	1.93	0.50
1:A:236:GLU:OE1	1:A:239:ARG:NH1	2.44	0.50
1:B:162:ASN:OD1	1:B:162:ASN:N	2.44	0.50
1:A:444:LYS:O	1:A:445:LEU:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:LEU:C	1:A:447:ASN:N	2.64	0.50
1:B:234:ASN:O	1:B:238:ARG:HB2	2.11	0.50
1:B:341:HIS:CD2	1:B:343:CYS:H	2.29	0.50
1:A:276:ARG:CZ	1:A:324:ILE:CD1	2.90	0.50
1:A:376:PRO:CB	1:A:377:VAL:CA	2.89	0.50
1:A:393:VAL:CG1	1:A:397:GLU:HA	2.42	0.50
1:A:276:ARG:HG3	1:A:382:TRP:CZ2	2.48	0.49
1:B:312:GLY:HA2	1:B:354:GLU:HA	1.94	0.49
1:A:78:LYS:HA	1:A:123:PHE:CE1	2.47	0.49
1:A:337:PRO:O	1:A:338:PRO:O	2.31	0.49
1:A:378:ASP:CB	1:A:380:THR:OG1	2.60	0.49
1:A:92:ALA:HA	1:A:200:LEU:HD12	1.94	0.49
1:A:372:PHE:CE1	1:A:377:VAL:HG13	2.47	0.49
1:A:229:THR:HG22	1:B:229:THR:HG22	1.94	0.49
1:A:320:ILE:HG22	1:A:334:ILE:HB	1.93	0.49
1:A:348:LEU:HD22	1:A:352:VAL:HG12	1.95	0.48
1:B:241:GLN:HE22	1:B:244:LEU:HD23	1.78	0.48
1:A:376:PRO:HB2	1:A:377:VAL:HA	1.92	0.48
1:B:123:PHE:O	1:B:126:ASN:N	2.46	0.48
1:A:121:SER:HB2	1:A:126:ASN:HD21	1.78	0.48
1:A:257:ILE:HA	1:A:436:THR:HG21	1.95	0.48
1:A:428:PHE:C	1:A:428:PHE:CD1	2.87	0.48
1:A:61:ILE:HD12	1:A:90:LEU:HD22	1.95	0.48
1:A:274:CYS:SG	1:A:405:PHE:HB3	2.54	0.48
1:B:255:THR:HA	1:B:439:TYR:CD1	2.49	0.47
1:A:313:ARG:CA	1:A:315:VAL:HG23	2.45	0.47
1:B:363:ASN:HB3	1:B:365:PRO:CD	2.44	0.47
1:A:251:PHE:HA	1:B:434:LEU:HD23	1.97	0.47
1:A:231:TYR:CE1	1:A:235:ILE:HD11	2.50	0.47
1:A:374:LYS:HB3	1:A:376:PRO:CG	2.45	0.47
1:B:152:PHE:CD1	1:B:152:PHE:C	2.89	0.46
1:B:262:HIS:O	1:B:263:LYS:C	2.53	0.46
1:B:92:ALA:HA	1:B:200:LEU:HD12	1.97	0.46
1:A:232:LEU:HD11	1:A:417:TYR:CZ	2.50	0.46
1:B:375:GLY:N	1:B:376:PRO:CD	2.78	0.46
1:A:405:PHE:N	1:A:405:PHE:CD1	2.82	0.46
1:B:257:ILE:HG23	1:B:258:GLU:N	2.31	0.46
1:B:320:ILE:HG22	1:B:337:PRO:HB3	1.96	0.46
1:B:55:ARG:HA	1:B:55:ARG:HE	1.79	0.46
1:A:238:ARG:O	1:A:242:MET:HG3	2.16	0.46
1:B:146:VAL:HG11	1:B:193:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:HB3	1:A:380:THR:H	1.79	0.46
1:A:97:SER:CB	1:A:115:LEU:HD23	2.46	0.46
1:A:129:ASN:HB3	1:A:131:ASP:OD1	2.16	0.46
1:A:51:LYS:O	1:A:54:SER:N	2.49	0.46
1:A:258:GLU:CG	1:A:259:ARG:N	2.79	0.46
1:A:91:LEU:O	1:A:92:ALA:C	2.55	0.45
1:A:209:ASP:O	1:A:210:GLU:C	2.54	0.45
1:B:277:TYR:CE2	1:B:325:LEU:HD11	2.51	0.45
1:B:365:PRO:O	1:B:367:ASP:N	2.50	0.45
1:A:248:ASN:HB2	1:B:431:TRP:CZ3	2.52	0.45
1:A:169:ASP:HB3	1:A:175:THR:HA	1.99	0.45
1:B:104:ARG:HG2	1:B:414:PHE:O	2.16	0.45
1:B:157:ASP:OD1	1:B:159:LYS:HD2	2.16	0.45
1:B:76:MET:O	1:B:80:VAL:HG23	2.15	0.45
1:A:283:ASP:HB2	1:A:316:ASN:HD22	1.82	0.45
1:A:166:ASP:O	1:A:170:LYS:HB3	2.17	0.45
1:A:313:ARG:C	1:A:315:VAL:HG23	2.37	0.45
1:B:390:LEU:N	1:B:390:LEU:HD12	2.31	0.45
1:B:363:ASN:CB	1:B:365:PRO:HD2	2.47	0.45
1:B:365:PRO:O	1:B:366:ALA:C	2.54	0.45
1:B:374:LYS:HB3	1:B:376:PRO:HD2	1.99	0.45
1:A:394:ASN:HB3	1:A:397:GLU:N	2.32	0.45
1:A:313:ARG:HA	1:A:315:VAL:HG23	1.99	0.44
1:B:141:GLY:HA2	1:B:165:SER:HB3	1.99	0.44
1:B:89:GLN:HB2	1:B:119:PRO:CG	2.48	0.44
1:A:207:LYS:O	1:A:211:GLU:HG2	2.16	0.44
1:B:103:SER:HA	1:B:108:PRO:HA	1.99	0.44
1:B:276:ARG:CD	1:B:324:ILE:HG13	2.48	0.44
1:B:348:LEU:HB3	1:B:349:PRO:HD3	2.00	0.44
1:B:276:ARG:HD3	1:B:324:ILE:HG13	2.00	0.44
1:A:351:TYR:O	1:A:354:GLU:HG2	2.18	0.44
1:B:362:MET:O	1:B:385:LYS:O	2.35	0.44
1:B:433:VAL:O	1:B:436:THR:HB	2.18	0.44
1:A:394:ASN:OD1	1:A:395:LYS:N	2.46	0.43
1:B:186:GLN:O	1:B:189:GLU:N	2.51	0.43
1:B:386:ASN:ND2	1:B:413:PRO:HA	2.33	0.43
1:B:398:GLU:HG3	1:B:399:ILE:H	1.83	0.43
1:B:435:ASN:N	1:B:435:ASN:OD1	2.51	0.43
1:A:182:ILE:CG2	1:A:217:LEU:HD13	2.48	0.43
1:A:245:TRP:O	1:A:248:ASN:N	2.51	0.43
1:A:348:LEU:HD13	1:A:389:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:SER:N	1:A:209:ASP:OD2	2.50	0.43
1:A:442:MET:HE1	1:B:441:LYS:HE3	2.00	0.43
1:B:363:ASN:HB3	1:B:365:PRO:HD3	2.00	0.43
1:A:65:LEU:HB3	1:A:219:PHE:CZ	2.54	0.43
1:B:139:ASP:C	1:B:140:ILE:HG13	2.39	0.43
1:B:180:MET:HE1	1:B:210:GLU:HG3	2.00	0.43
1:B:364:ALA:N	1:B:365:PRO:CD	2.82	0.43
1:A:149:THR:O	1:A:150:LYS:HG2	2.19	0.43
1:A:166:ASP:O	1:A:170:LYS:CB	2.66	0.43
1:B:123:PHE:HZ	1:B:127:LEU:HD13	1.83	0.43
1:A:120:THR:O	1:A:121:SER:C	2.57	0.43
1:A:320:ILE:CG2	1:A:334:ILE:HB	2.48	0.43
1:B:255:THR:HA	1:B:439:TYR:CE1	2.54	0.43
1:A:372:PHE:CG	1:A:377:VAL:HG22	2.54	0.42
1:B:186:GLN:O	1:B:187:GLY:C	2.57	0.42
1:B:255:THR:OG1	1:B:256:ASP:N	2.51	0.42
1:A:262:HIS:CD2	1:A:321:ILE:HD11	2.55	0.42
1:B:69:ILE:O	1:B:70:GLN:C	2.56	0.42
1:A:262:HIS:HA	1:A:323:TYR:OH	2.19	0.42
1:B:422:ILE:O	1:B:426:THR:HG23	2.19	0.42
1:A:97:SER:HB2	1:A:115:LEU:HD23	2.00	0.42
1:B:123:PHE:C	1:B:123:PHE:CD2	2.92	0.42
1:A:360:ASN:OD1	1:A:360:ASN:C	2.58	0.42
1:B:360:ASN:HD21	1:B:414:PHE:C	2.22	0.42
1:B:415:ASP:C	1:B:415:ASP:OD1	2.58	0.42
1:A:95:ARG:O	1:A:197:LEU:HB2	2.19	0.42
1:A:69:ILE:CD1	1:A:223:VAL:HG22	2.48	0.42
1:B:159:LYS:HE2	1:B:159:LYS:N	2.35	0.42
1:B:265:LEU:HB2	1:B:323:TYR:OH	2.20	0.42
1:A:320:ILE:HD13	1:A:341:HIS:CD2	2.55	0.42
1:B:398:GLU:CG	1:B:399:ILE:N	2.83	0.41
1:B:123:PHE:CZ	1:B:127:LEU:HB2	2.55	0.41
1:B:276:ARG:HB2	1:B:406:TYR:HB2	2.02	0.41
1:B:184:ILE:HD12	1:B:224:LEU:HD22	2.03	0.41
1:A:107:ILE:HG22	1:A:108:PRO:O	2.20	0.41
1:A:131:ASP:N	1:A:131:ASP:OD1	2.53	0.41
1:A:261:PHE:O	1:A:262:HIS:C	2.59	0.41
1:A:84:LEU:HD22	1:A:96:CYS:CB	2.51	0.41
1:B:389:SER:HB2	1:B:404:THR:OG1	2.21	0.41
1:A:75:SER:O	1:A:76:MET:C	2.59	0.41
1:B:249:LYS:O	1:B:250:VAL:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:LEU:C	1:A:447:ASN:H	2.24	0.41
1:A:84:LEU:HD22	1:A:96:CYS:HB3	2.03	0.41
1:B:232:LEU:HD11	1:B:417:TYR:CZ	2.56	0.41
1:A:199:LYS:HG3	1:A:202:ALA:HB3	2.02	0.41
1:A:243:LEU:O	1:A:244:LEU:C	2.58	0.41
1:A:341:HIS:CE1	1:A:342:TRP:CD1	3.08	0.41
1:A:348:LEU:O	1:A:351:TYR:N	2.54	0.41
1:A:191:LEU:CD2	1:A:228:HIS:CD2	3.04	0.41
1:A:365:PRO:O	1:A:366:ALA:C	2.59	0.41
1:B:393:VAL:HG13	1:B:398:GLU:O	2.21	0.41
1:A:348:LEU:CD2	1:A:352:VAL:HG12	2.51	0.40
1:A:276:ARG:NH1	1:A:324:ILE:HD13	2.35	0.40
1:A:239:ARG:HB2	1:A:421:ILE:HG22	2.03	0.40
1:A:232:LEU:HB3	1:B:233:TYR:CE1	2.56	0.40
1:B:310:PRO:CB	1:B:311:ASP:HA	2.51	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	378/862 (44%)	299 (79%)	56 (15%)	23 (6%)	1	12
1	B	371/862 (43%)	300 (81%)	53 (14%)	18 (5%)	2	17
All	All	749/1724 (43%)	599 (80%)	109 (15%)	41 (6%)	2	14

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ILE
1	A	312	GLY
1	A	338	PRO

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Mol	Chain	Res	Type
1	A	362	MET
1	A	367	ASP
1	A	374	LYS
1	A	394	ASN
1	B	60	ASN
1	B	174	TYR
1	B	313	ARG
1	B	416	GLU
1	A	75	SER
1	A	198	ASN
1	A	366	ALA
1	A	376	PRO
1	A	397	GLU
1	A	407	ASN
1	B	198	ASN
1	B	394	ASN
1	A	156	PRO
1	B	85	GLN
1	B	315	VAL
1	B	345	ILE
1	B	366	ALA
1	B	376	PRO
1	B	407	ASN
1	A	120	THR
1	A	177	VAL
1	A	316	ASN
1	B	108	PRO
1	B	213	PHE
1	B	316	ASN
1	B	335	PRO
1	A	113	ARG
1	A	267	THR
1	A	446	GLU
1	B	59	CYS
1	B	436	THR
1	A	364	ALA
1	A	452	ALA
1	A	321	ILE

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	347/773 (45%)	308 (89%)	39 (11%)	6 25
1	B	340/773 (44%)	305 (90%)	35 (10%)	7 29
All	All	687/1546 (44%)	613 (89%)	74 (11%)	6 27

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	66	LEU
1	A	71	ASP
1	A	79	ILE
1	A	83	THR
1	A	120	THR
1	A	121	SER
1	A	140	ILE
1	A	150	LYS
1	A	160	LYS
1	A	161	ASN
1	A	166	ASP
1	A	172	THR
1	A	175	THR
1	A	177	VAL
1	A	180	MET
1	A	206	SER
1	A	208	GLU
1	A	232	LEU
1	A	237	SER
1	A	243	LEU
1	A	244	LEU
1	A	255	THR
1	A	258	GLU
1	A	267	THR
1	A	272	LEU
1	A	345	ILE

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Mol	Chain	Res	Type
1	A	348	LEU
1	A	352	VAL
1	A	355	ASN
1	A	360	ASN
1	A	362	MET
1	A	370	PHE
1	A	373	GLN
1	A	374	LYS
1	A	390	LEU
1	A	426	THR
1	A	442	MET
1	A	448	ARG
1	B	60	ASN
1	B	75	SER
1	B	82	LYS
1	B	102	ARG
1	B	103	SER
1	B	112	THR
1	B	122	LYS
1	B	127	LEU
1	B	131	ASP
1	B	159	LYS
1	B	162	ASN
1	B	165	SER
1	B	166	ASP
1	B	171	LYS
1	B	179	MET
1	B	185	THR
1	B	217	LEU
1	B	232	LEU
1	B	240	SER
1	B	243	LEU
1	B	254	LEU
1	B	259	ARG
1	B	274	CYS
1	B	276	ARG
1	B	284	MET
1	B	314	GLU
1	B	319	LYS
1	B	336	THR
1	B	368	GLU
1	B	373	GLN

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Mol	Chain	Res	Type
1	B	379	GLU
1	B	380	THR
1	B	383	VAL
1	B	442	MET
1	B	445	LEU

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	89	GLN
1	A	105	ASN
1	A	126	ASN
1	A	186	GLN
1	A	228	HIS
1	A	260	GLN
1	A	262	HIS
1	A	316	ASN
1	A	341	HIS
1	A	373	GLN
1	B	105	ASN
1	B	126	ASN
1	B	163	HIS
1	B	228	HIS
1	B	241	GLN
1	B	316	ASN
1	B	341	HIS
1	B	386	ASN
1	B	420	GLN

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

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	382/862 (44%)	-0.26	4 (1%)	82	72	39, 70, 109, 128	0
1	B	375/862 (43%)	-0.21	5 (1%)	77	65	33, 69, 115, 133	0
All	All	757/1724 (43%)	-0.23	9 (1%)	79	67	33, 70, 113, 133	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	453	GLN	4.8
1	B	448	ARG	3.4
1	A	453	GLN	3.2
1	A	451	ILE	3.2
1	B	203	SER	2.8
1	A	452	ALA	2.7
1	B	375	GLY	2.4
1	A	372	PHE	2.2
1	B	202	ALA	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.