Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:02 PM GMT

PDB ID	:	4E6X
Title	:	ClbP in complex boron-based inhibitor
Authors	:	Cougnoux, A.; Delmas, J.; Bonnet, R.
Deposited on	:	2012-03-16
Resolution	:	2.24 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

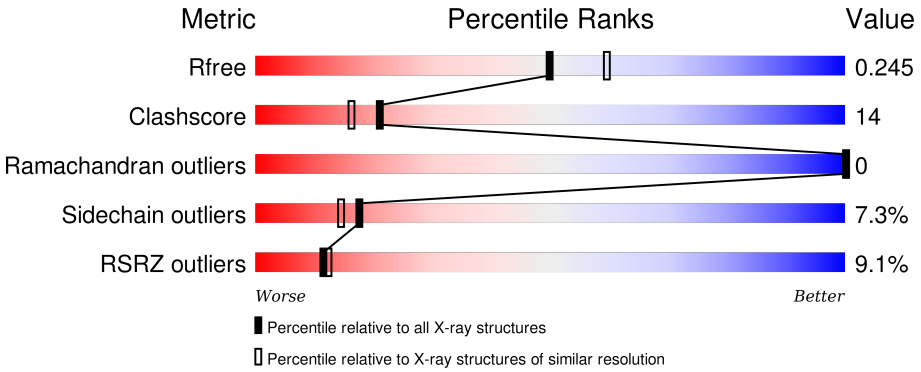
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.24 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}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	336	8% 68% 21% • 8%
1	B	336	8% 68% 19% • 10%
1	C	336	8% 70% 18% • 9%

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
2	PO4	A	401	-	-	-	X

2 Entry composition

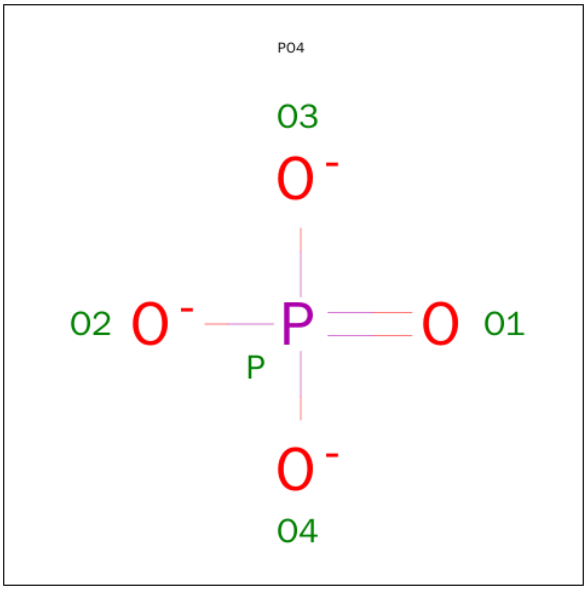
There are 4 unique types of molecules in this entry. The entry contains 7261 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ClbP peptidase.

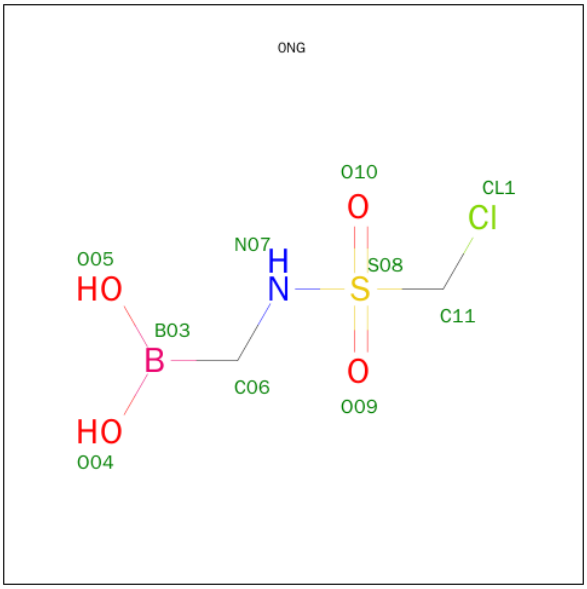
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	2	0
			2383	1516	415	443	9			
1	B	301	Total	C	N	O	S	0	0	0
			2321	1484	399	429	9			
1	C	305	Total	C	N	O	S	0	1	0
			2350	1501	405	435	9			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is ({[(CHLOROMETHYL)SULFONYL]AMINO}METHYL)BORONIC ACID (three-letter code: 0NG) (formula: $C_2H_7BClNO_4S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	B	1	Total	B	C	Cl	N	O	S	0	0
			10	1	2	1	1	4	1		
3	C	1	Total	B	C	Cl	N	O	S	0	0
			10	1	2	1	1	4	1		

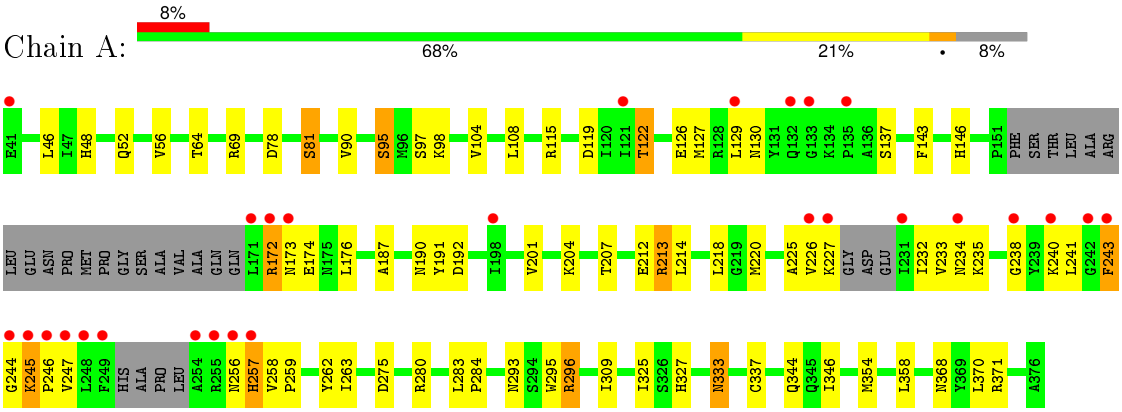
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	49	Total	O	0	0
			49	49		
4	C	62	Total	O	0	0
			62	62		

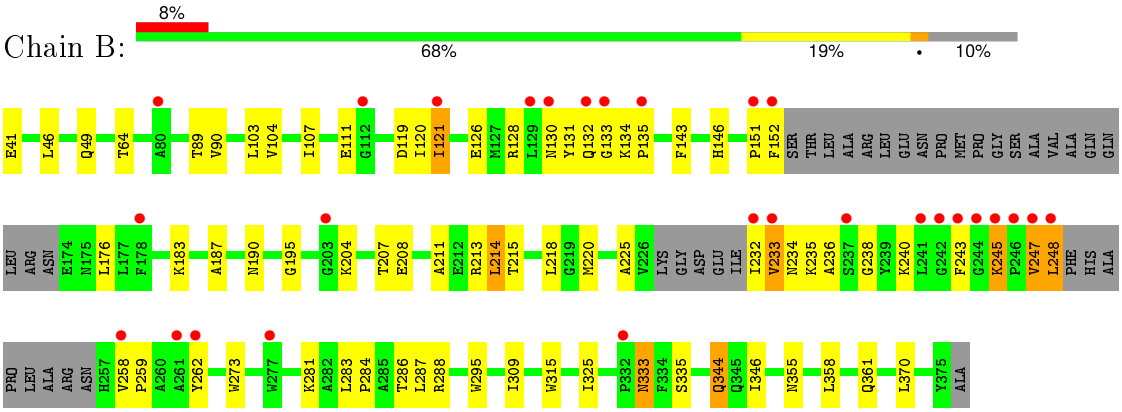
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

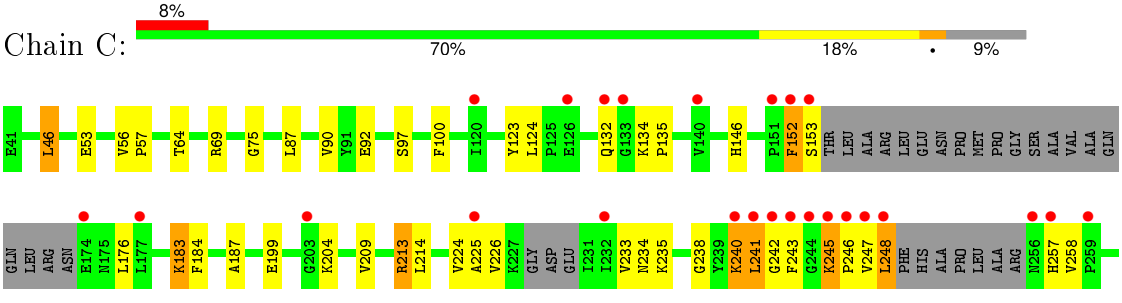
- Molecule 1: ClbP peptidase

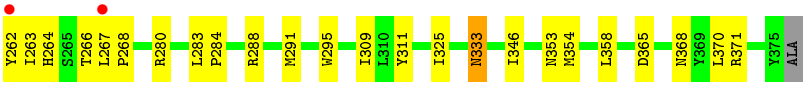


- Molecule 1: ClbP peptidase



- Molecule 1: ClbP peptidase




Y262
I263
H264
S265
T266
L267
P268
R280
L283
P284
R288
M291
W295
I309
L310
Y311
I325
N333
I346
N353
M354
L358
D365
N368
Y369
L370
R371
Y375
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.05Å 152.53Å 86.89Å 90.00° 123.43° 90.00°	Depositor
Resolution (Å)	52.55 – 2.24 52.55 – 2.24	Depositor EDS
% Data completeness (in resolution range)	79.0 (52.55-2.24) 78.0 (52.55-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.200 , 0.249 0.195 , 0.245	Depositor DCC
R_{free} test set	2776 reflections (6.77%)	DCC
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 27.9	EDS
Estimated twinning fraction	0.467 for 1/2*h+1/2*k+l,3/2*h-1/2*k+l,-l 0.459 for 1/2*h-1/2*k+l,-3/2*h-1/2*k-l,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 43180 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7261	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, 0NG

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	0.71	1/2435 (0.0%)	0.83	0/3308
1	B	0.60	0/2368	0.81	1/3217 (0.0%)
1	C	0.60	0/2400	0.79	0/3262
All	All	0.64	1/7203 (0.0%)	0.81	1/9787 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	337	CYS	CB-SG	-5.68	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	183	LYS	CB-CA-C	-5.13	100.13	110.40

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	2383	0	2370	58	0
1	B	2321	0	2321	75	0
1	C	2350	0	2341	69	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
3	B	10	0	5	0	0
3	C	10	0	5	0	0
4	A	61	0	0	0	0
4	B	49	0	0	0	0
4	C	62	0	0	0	0
All	All	7261	0	7042	202	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 14.

All (202) 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:C:152:PHE:HD1	1:C:152:PHE:C	1.52	1.12
1:A:283:LEU:HB3	1:A:284:PRO:HD2	1.29	1.08
1:C:134:LYS:HG2	1:C:135:PRO:HD2	1.30	1.07
1:B:344:GLN:O	1:B:344:GLN:HG3	1.57	1.04
1:C:152:PHE:CD1	1:C:152:PHE:C	2.29	1.02
1:C:245:LYS:O	1:C:245:LYS:HG2	1.55	1.02
1:C:152:PHE:O	1:C:152:PHE:HD1	1.49	0.94
1:A:243:PHE:N	1:A:243:PHE:HD1	1.67	0.92
1:C:134:LYS:HG2	1:C:135:PRO:CD	2.00	0.90
1:A:333:ASN:HD22	1:A:333:ASN:H	1.16	0.90
1:A:243:PHE:CD1	1:A:243:PHE:N	2.39	0.88
1:C:46:LEU:O	1:C:46:LEU:HD23	1.72	0.87
1:A:245:LYS:O	1:A:245:LYS:HD3	1.74	0.86
1:C:152:PHE:O	1:C:152:PHE:CD1	2.29	0.83
1:A:333:ASN:H	1:A:333:ASN:ND2	1.75	0.83
1:B:248:LEU:CD1	1:B:248:LEU:C	2.46	0.83
1:B:245:LYS:CD	1:B:245:LYS:O	2.29	0.80
1:A:172:ARG:HG2	1:A:173:ASN:N	1.96	0.79
1:C:46:LEU:CD2	1:C:46:LEU:O	2.30	0.78
1:B:245:LYS:CG	1:B:245:LYS:O	2.31	0.78
1:C:134:LYS:CG	1:C:135:PRO:HD2	2.10	0.78
1:A:283:LEU:HB3	1:A:284:PRO:CD	2.11	0.77
1:A:245:LYS:CG	1:A:245:LYS:O	2.32	0.77
1:B:90:VAL:HB	1:B:235:LYS:HA	1.66	0.76
1:C:90:VAL:HB	1:C:235:LYS:HA	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:VAL:HA	1:B:262:TYR:HB2	1.69	0.75
1:C:241:LEU:O	1:C:241:LEU:HD23	1.86	0.75
1:A:280:ARG:HH11	1:A:280:ARG:HG2	1.51	0.75
1:B:258:VAL:HG13	1:B:262:TYR:O	1.88	0.74
1:C:245:LYS:O	1:C:245:LYS:CG	2.34	0.74
1:A:309:ILE:HB	2:A:401:PO4:O1	1.87	0.73
1:B:146:HIS:CD2	1:B:187:ALA:H	2.07	0.73
1:B:220:MET:HE1	1:B:273:TRP:HE3	1.54	0.73
1:A:245:LYS:CD	1:A:245:LYS:O	2.36	0.72
1:B:146:HIS:HD2	1:B:187:ALA:H	1.37	0.72
1:B:89:THR:CG2	1:B:236:ALA:HB2	2.19	0.72
1:B:240:LYS:HZ2	1:B:248:LEU:HD23	1.54	0.71
1:C:46:LEU:CD2	1:C:46:LEU:C	2.59	0.71
1:A:146:HIS:CD2	1:A:187:ALA:H	2.08	0.71
1:B:240:LYS:NZ	1:B:248:LEU:HD23	2.07	0.70
1:B:245:LYS:HD3	1:B:245:LYS:O	1.92	0.70
1:C:280:ARG:O	1:C:288:ARG:HG3	1.92	0.69
1:C:240:LYS:O	1:C:246:PRO:HD2	1.92	0.69
1:A:97:SER:HB3	1:A:263:ILE:HD12	1.74	0.69
1:A:232:ILE:HG22	1:A:233:VAL:O	1.93	0.69
1:B:248:LEU:HD13	1:B:248:LEU:C	2.13	0.68
1:C:283:LEU:HB3	1:C:284:PRO:HD2	1.76	0.67
1:C:248:LEU:HB3	1:C:333:ASN:HD22	1.60	0.67
1:A:146:HIS:HD2	1:A:187:ALA:H	1.42	0.65
1:A:245:LYS:HG2	1:A:245:LYS:O	1.96	0.65
1:B:248:LEU:HD12	1:B:248:LEU:C	2.17	0.63
1:A:243:PHE:H	1:A:243:PHE:HD1	1.29	0.63
1:C:92:GLU:HG2	1:C:264:HIS:NE2	2.14	0.63
1:B:245:LYS:O	1:B:245:LYS:HG2	1.99	0.62
1:B:151:PRO:O	1:B:152:PHE:HB2	1.97	0.62
1:C:57:PRO:HD3	1:C:354:MET:HE3	1.81	0.62
1:A:119:ASP:O	1:A:122:THR:HG23	1.99	0.62
1:C:245:LYS:O	1:C:245:LYS:HE2	2.00	0.61
1:C:257:HIS:HD2	1:C:262:TYR:HE2	1.49	0.60
1:B:218:LEU:HD13	1:B:220:MET:CE	2.32	0.60
1:B:248:LEU:HD13	1:B:248:LEU:O	2.03	0.59
1:A:226:VAL:O	1:A:258:VAL:HG21	2.02	0.58
1:A:280:ARG:HG2	1:A:280:ARG:NH1	2.16	0.58
1:B:248:LEU:HD12	1:B:333:ASN:ND2	2.19	0.58
1:B:233:VAL:O	1:B:234:ASN:HB2	2.02	0.57
1:B:309:ILE:HB	2:B:401:PO4:O1	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HE3	1:A:212:GLU:OE1	2.04	0.57
1:C:92:GLU:HG2	1:C:264:HIS:CD2	2.40	0.57
1:A:333:ASN:ND2	1:A:333:ASN:N	2.42	0.57
1:C:233:VAL:O	1:C:234:ASN:HB2	2.04	0.56
1:A:129:LEU:HD23	1:A:174:GLU:HB3	1.86	0.56
1:C:146:HIS:CD2	1:C:187:ALA:H	2.23	0.56
1:C:97:SER:HB3	1:C:263:ILE:HD12	1.88	0.56
1:B:46:LEU:HD23	1:B:46:LEU:O	2.05	0.56
1:B:143:PHE:HD1	1:B:190:ASN:HD22	1.55	0.55
1:A:293:ASN:HA	1:A:296:ARG:HE	1.71	0.55
1:A:226:VAL:HG23	1:A:226:VAL:O	2.07	0.55
1:B:218:LEU:HD13	1:B:220:MET:HE3	1.89	0.54
1:A:143:PHE:HD1	1:A:190:ASN:HD22	1.55	0.54
1:A:207:THR:HG23	1:A:225:ALA:O	2.07	0.54
1:C:46:LEU:HD23	1:C:46:LEU:C	2.26	0.54
1:B:220:MET:HE2	1:B:273:TRP:CA	2.38	0.54
1:A:333:ASN:HD22	1:A:333:ASN:N	1.85	0.54
1:C:248:LEU:HB3	1:C:333:ASN:ND2	2.22	0.54
1:C:368:ASN:HD22	1:C:371:ARG:HH21	1.56	0.54
1:B:238:GLY:HA3	1:B:333:ASN:HB2	1.89	0.54
1:A:64:THR:HB	1:A:69:ARG:HG3	1.90	0.53
1:C:257:HIS:HD2	1:C:262:TYR:CE2	2.26	0.53
1:C:240:LYS:HZ2	1:C:248:LEU:CD1	2.21	0.53
1:B:248:LEU:HD12	1:B:333:ASN:HD21	1.74	0.53
1:B:104:VAL:HG23	1:B:214:LEU:HD22	1.91	0.52
1:B:245:LYS:C	1:B:245:LYS:HD3	2.29	0.52
1:B:358:LEU:N	1:B:358:LEU:HD12	2.24	0.52
1:C:46:LEU:HD22	1:C:46:LEU:C	2.29	0.52
1:C:134:LYS:CG	1:C:135:PRO:CD	2.81	0.52
1:B:344:GLN:HG2	1:B:346:ILE:CD1	2.39	0.52
1:B:131:TYR:O	1:B:132:GLN:HB2	2.09	0.52
1:B:315:TRP:CE3	1:B:325:ILE:HG22	2.45	0.52
1:B:295:TRP:CZ3	1:B:325:ILE:HD13	2.45	0.51
1:C:56:VAL:HG12	1:C:354:MET:HB3	1.91	0.51
1:B:344:GLN:HG2	1:B:346:ILE:HD11	1.93	0.51
1:C:258:VAL:HA	1:C:262:TYR:HB2	1.92	0.51
1:A:258:VAL:HA	1:A:262:TYR:HB2	1.92	0.51
1:B:121:ILE:HG23	1:B:121:ILE:O	2.10	0.51
1:B:220:MET:HE2	1:B:273:TRP:HA	1.93	0.51
1:C:184:PHE:CE2	1:C:311:TYR:HB2	2.46	0.50
1:C:226:VAL:O	1:C:258:VAL:HG21	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:MET:HE1	1:B:273:TRP:CE3	2.41	0.50
1:B:283:LEU:HB3	1:B:284:PRO:HD2	1.93	0.50
1:B:89:THR:HG21	1:B:236:ALA:HB2	1.92	0.50
1:C:123:TYR:O	1:C:124:LEU:HD12	2.12	0.50
1:A:192:ASP:OD1	1:A:257:HIS:HA	2.12	0.50
1:A:218:LEU:HB2	1:A:220:MET:HE2	1.92	0.49
1:B:240:LYS:NZ	1:B:248:LEU:CD2	2.74	0.49
1:A:244:GLY:O	1:A:246:PRO:HD3	2.13	0.49
1:B:281:LYS:HA	1:B:288:ARG:HD2	1.95	0.49
1:A:78:ASP:OD2	1:A:81:SER:HB3	2.13	0.49
1:B:207:THR:HG23	1:B:225:ALA:O	2.13	0.49
1:C:209:VAL:O	1:C:213:ARG:HB2	2.13	0.49
1:C:309:ILE:HB	2:C:401:PO4:O2	2.13	0.49
1:C:46:LEU:O	1:C:46:LEU:HD22	2.12	0.48
1:C:134:LYS:HG2	1:C:135:PRO:N	2.28	0.48
1:B:335:SER:HB3	1:B:355:ASN:HA	1.95	0.48
1:B:220:MET:CE	1:B:273:TRP:HA	2.43	0.48
1:C:123:TYR:C	1:C:124:LEU:HD12	2.34	0.48
1:C:240:LYS:HZ2	1:C:248:LEU:CD2	2.27	0.48
1:A:56:VAL:HG12	1:A:354:MET:HB3	1.96	0.47
1:A:238:GLY:HA3	1:A:333:ASN:HB2	1.97	0.47
1:C:241:LEU:CD2	1:C:241:LEU:O	2.61	0.47
1:B:245:LYS:HD3	1:B:245:LYS:N	2.29	0.47
1:C:241:LEU:HG	1:C:242:GLY:O	2.15	0.47
1:C:266:THR:HB	1:C:268:PRO:HD2	1.96	0.47
1:B:238:GLY:HA3	1:B:333:ASN:CB	2.44	0.47
1:A:233:VAL:HG23	1:A:234:ASN:OD1	2.15	0.47
1:A:368:ASN:HD22	1:A:371:ARG:HH21	1.62	0.47
1:A:127:MET:O	1:A:127:MET:HG2	2.15	0.47
1:B:64:THR:O	1:B:346:ILE:HA	2.15	0.46
1:B:218:LEU:HD13	1:B:220:MET:HE1	1.97	0.46
1:C:333:ASN:N	1:C:333:ASN:OD1	2.48	0.46
1:B:247:VAL:CG2	1:B:248:LEU:N	2.78	0.46
1:B:333:ASN:N	1:B:333:ASN:OD1	2.48	0.46
1:A:95:SER:HG	1:A:98:LYS:HZ3	1.62	0.46
1:C:283:LEU:HB3	1:C:284:PRO:CD	2.44	0.46
1:C:368:ASN:ND2	1:C:371:ARG:HH21	2.14	0.46
1:C:267:LEU:HB3	1:C:268:PRO:HD3	1.97	0.46
1:B:204:LYS:HB3	1:B:208:GLU:OE1	2.16	0.46
1:B:103:LEU:O	1:B:107:ILE:HG13	2.16	0.46
1:A:95:SER:OG	1:A:98:LYS:NZ	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ILE:HD12	1:B:232:ILE:N	2.31	0.45
1:B:103:LEU:HD23	1:B:214:LEU:HD11	1.99	0.45
1:B:245:LYS:H	1:B:245:LYS:HD3	1.81	0.45
1:A:172:ARG:HG2	1:A:173:ASN:H	1.76	0.45
1:C:64:THR:O	1:C:346:ILE:HA	2.16	0.45
1:B:361:GLN:HG3	1:B:361:GLN:O	2.16	0.45
1:A:191:TYR:O	1:A:259:PRO:HB2	2.17	0.45
1:A:104:VAL:HG23	1:A:214:LEU:HD11	1.98	0.45
1:A:64:THR:O	1:A:346:ILE:HA	2.16	0.44
1:A:95:SER:HB3	1:A:327:HIS:CE1	2.52	0.44
1:A:283:LEU:CB	1:A:284:PRO:HD2	2.18	0.44
1:B:238:GLY:C	1:B:333:ASN:HB3	2.38	0.44
1:B:130:ASN:OD1	1:B:135:PRO:HA	2.18	0.44
1:B:286:THR:HG23	1:B:287:LEU:N	2.33	0.44
1:B:132:GLN:HB3	1:B:133:GLY:H	1.47	0.44
1:C:213:ARG:HA	1:C:213:ARG:HD2	1.71	0.44
1:A:240:LYS:O	1:A:246:PRO:HD2	2.18	0.43
1:C:46:LEU:HD11	1:C:365:ASP:HB3	1.99	0.43
1:C:224:VAL:HG22	1:C:225:ALA:N	2.34	0.43
1:A:295:TRP:CE3	1:A:325:ILE:HD13	2.53	0.43
1:C:152:PHE:CD1	1:C:153:SER:N	2.85	0.43
1:B:211:ALA:HA	1:B:215:THR:OG1	2.18	0.43
1:A:48:HIS:O	1:A:52:GLN:HG3	2.17	0.43
1:B:214:LEU:HA	1:B:214:LEU:HD12	1.79	0.43
1:B:119:ASP:OD1	1:B:120:ILE:N	2.51	0.43
1:C:224:VAL:HG13	1:C:224:VAL:O	2.19	0.43
1:C:280:ARG:HB2	1:C:291:MET:SD	2.59	0.43
1:C:238:GLY:HA3	1:C:333:ASN:HB2	2.00	0.43
1:C:199:GLU:HG2	1:C:204:LYS:O	2.18	0.42
1:C:262:TYR:O	1:C:264:HIS:ND1	2.52	0.42
1:A:90:VAL:HB	1:A:235:LYS:HA	2.00	0.42
1:A:69:ARG:NH2	1:A:275:ASP:OD2	2.52	0.42
1:C:64:THR:HB	1:C:69:ARG:HG3	2.01	0.42
1:C:152:PHE:HD1	1:C:153:SER:N	2.11	0.42
1:B:195:GLY:HA3	1:B:259:PRO:HG2	2.01	0.42
1:A:233:VAL:O	1:A:234:ASN:HB2	2.18	0.42
1:A:108:LEU:HD13	1:A:201:VAL:HG11	2.02	0.42
1:B:90:VAL:N	1:B:234:ASN:O	2.25	0.42
1:B:134:LYS:H	1:B:134:LYS:HG3	1.68	0.42
1:C:57:PRO:HD2	1:C:353:ASN:OD1	2.20	0.42
1:B:46:LEU:HD23	1:B:46:LEU:C	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:N	1:A:213:ARG:HD2	2.34	0.41
1:B:111:GLU:CD	1:B:213:ARG:HH22	2.23	0.41
1:A:130:ASN:N	1:A:174:GLU:O	2.38	0.41
1:B:281:LYS:HA	1:B:288:ARG:CD	2.50	0.41
1:C:183:LYS:HB2	1:C:183:LYS:HE3	1.61	0.41
1:C:57:PRO:O	1:C:75:GLY:HA3	2.21	0.41
1:C:87:LEU:HD23	1:C:87:LEU:HA	1.93	0.41
1:A:245:LYS:HB2	1:A:354:MET:HE2	2.02	0.41
1:B:46:LEU:C	1:B:46:LEU:CD2	2.89	0.41
1:B:295:TRP:CE3	1:B:325:ILE:HD13	2.55	0.41
1:C:295:TRP:CZ3	1:C:325:ILE:HD13	2.56	0.40
1:C:100:PHE:HB2	1:C:263:ILE:CD1	2.51	0.40
1:B:134:LYS:HB3	1:B:135:PRO:HD2	2.02	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	304/336 (90%)	296 (97%)	8 (3%)	0	100	100
1	B	293/336 (87%)	281 (96%)	12 (4%)	0	100	100
1	C	298/336 (89%)	289 (97%)	9 (3%)	0	100	100
All	All	895/1008 (89%)	866 (97%)	29 (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	251/276 (91%)	228 (91%)	23 (9%)	11 8
1	B	247/276 (90%)	232 (94%)	15 (6%)	23 22
1	C	249/276 (90%)	232 (93%)	17 (7%)	20 17
All	All	747/828 (90%)	692 (93%)	55 (7%)	17 14

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	81	SER
1	A	95	SER
1	A	115	ARG
1	A	122	THR
1	A	126	GLU
1	A	137	SER
1	A	172	ARG
1	A	176	LEU
1	A	213	ARG
1	A	227	LYS
1	A	241	LEU
1	A	243	PHE
1	A	245	LYS
1	A	247	VAL
1	A	256[A]	ASN
1	A	256[B]	ASN
1	A	257	HIS
1	A	296	ARG
1	A	333	ASN
1	A	344	GLN
1	A	358	LEU
1	A	370	LEU
1	B	41	GLU
1	B	49	GLN
1	B	121	ILE
1	B	126	GLU
1	B	128	ARG
1	B	176	LEU
1	B	214	LEU
1	B	233	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	243	PHE
1	B	245	LYS
1	B	247	VAL
1	B	248	LEU
1	B	333	ASN
1	B	344	GLN
1	B	370	LEU
1	C	46	LEU
1	C	53	GLU
1	C	132	GLN
1	C	152	PHE
1	C	176	LEU
1	C	183	LYS
1	C	213	ARG
1	C	214	LEU
1	C	240	LYS
1	C	241	LEU
1	C	243	PHE
1	C	245	LYS
1	C	247	VAL
1	C	248	LEU
1	C	333	ASN
1	C	358	LEU
1	C	370	LEU

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

Mol	Chain	Res	Type
1	A	49	GLN
1	A	116	GLN
1	A	132	GLN
1	A	146	HIS
1	A	190	ASN
1	A	333	ASN
1	A	368	ASN
1	B	49	GLN
1	B	146	HIS
1	B	190	ASN
1	B	321	GLN
1	B	357	ASN
1	B	368	ASN
1	C	116	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	132	GLN
1	C	146	HIS
1	C	190	ASN
1	C	368	ASN

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

5 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	PO4	A	401	-	4,4,4	0.49	0	6,6,6	0.31	0
3	0NG	B	400	1	5,9,9	5.51	4 (80%)	6,12,12	2.92	3 (50%)
2	PO4	B	401	-	4,4,4	0.42	0	6,6,6	0.29	0
3	0NG	C	400	1	5,9,9	5.76	4 (80%)	6,12,12	3.02	3 (50%)
2	PO4	C	401	-	4,4,4	0.63	0	6,6,6	0.25	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
2	PO4	A	401	-	-	0/0/0/0	0/0/0/0
3	0NG	B	400	1	-	0/5/9/9	0/0/0/0
2	PO4	B	401	-	-	0/0/0/0	0/0/0/0
3	0NG	C	400	1	-	0/5/9/9	0/0/0/0
2	PO4	C	401	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	0NG	C06-N07	2.15	1.49	1.47
3	C	400	0NG	C06-N07	2.27	1.50	1.47
3	C	400	0NG	O10-S08	5.96	1.53	1.43
3	C	400	0NG	O09-S08	6.31	1.53	1.43
3	B	400	0NG	O10-S08	6.46	1.53	1.43
3	B	400	0NG	O09-S08	6.99	1.54	1.43
3	B	400	0NG	S08-N07	7.45	1.81	1.60
3	C	400	0NG	S08-N07	9.05	1.85	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	400	0NG	O09-S08-O10	-5.94	109.07	119.34
3	B	400	0NG	O09-S08-O10	-5.37	110.07	119.34
3	B	400	0NG	C06-N07-S08	-3.76	109.68	121.53
3	C	400	0NG	C06-N07-S08	-2.43	113.86	121.53
3	B	400	0NG	O10-S08-N07	2.86	113.68	106.91
3	C	400	0NG	O10-S08-N07	3.57	115.35	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PO4	1	0
2	B	401	PO4	1	0
2	C	401	PO4	1	0

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	310/336 (92%)	0.75	28 (9%)	12	12	17, 35, 74, 97	0
1	B	301/336 (89%)	0.77	28 (9%)	11	12	19, 34, 74, 101	0
1	C	305/336 (90%)	0.71	27 (8%)	12	13	19, 33, 73, 97	0
All	All	916/1008 (90%)	0.74	83 (9%)	11	12	17, 34, 74, 101	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	GLY	15.7
1	A	249	PHE	11.6
1	C	242	GLY	10.8
1	A	244	GLY	10.5
1	A	243	PHE	10.5
1	C	243	PHE	10.1
1	A	173	ASN	9.8
1	A	242	GLY	9.7
1	C	153	SER	9.0
1	B	152	PHE	7.7
1	C	247	VAL	7.4
1	A	234	ASN	7.3
1	A	247	VAL	7.3
1	B	243	PHE	6.9
1	B	247	VAL	6.7
1	C	174	GLU	6.6
1	C	152	PHE	6.6
1	A	238	GLY	6.5
1	A	245	LYS	6.2
1	B	248	LEU	5.7
1	A	246	PRO	5.6
1	C	246	PRO	5.5
1	A	255	ARG	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	246	PRO	5.1
1	B	245	LYS	5.0
1	A	41	GLU	4.8
1	A	257	HIS	4.6
1	B	151	PRO	4.5
1	B	262	TYR	4.2
1	A	133	GLY	4.1
1	C	267	LEU	4.0
1	C	241	LEU	4.0
1	C	259	PRO	3.9
1	C	245	LYS	3.9
1	B	261	ALA	3.8
1	B	242	GLY	3.8
1	C	257	HIS	3.7
1	C	244	GLY	3.6
1	B	237	SER	3.6
1	C	248	LEU	3.5
1	C	133	GLY	3.4
1	A	240	LYS	3.4
1	A	227	LYS	3.4
1	B	133	GLY	3.3
1	A	135	PRO	3.3
1	B	233	VAL	3.3
1	B	135	PRO	3.3
1	A	254	ALA	3.3
1	B	112	GLY	3.2
1	A	198	ILE	3.2
1	B	203	GLY	3.1
1	B	178	PHE	3.1
1	C	256	ASN	3.0
1	C	262	TYR	3.0
1	A	256[A]	ASN	3.0
1	A	231	ILE	3.0
1	A	129	LEU	2.9
1	C	203	GLY	2.9
1	B	129	LEU	2.8
1	C	225	ALA	2.8
1	B	232	ILE	2.7
1	C	177	LEU	2.6
1	C	240	LYS	2.6
1	B	130	ASN	2.6
1	A	172	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	2.5
1	B	332	PRO	2.5
1	A	226	VAL	2.4
1	A	248	LEU	2.3
1	C	120	ILE	2.3
1	C	132	GLN	2.3
1	C	151	PRO	2.2
1	B	121	ILE	2.2
1	B	241	LEU	2.2
1	B	277	TRP	2.1
1	B	132	GLN	2.1
1	A	121	ILE	2.1
1	A	132	GLN	2.1
1	B	80	ALA	2.1
1	C	140	VAL	2.1
1	C	126	GLU	2.0
1	C	232	ILE	2.0
1	B	258	VAL	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 carbohydrates 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. 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, 95^{th} 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
2	PO4	A	401	5/5	0.92	0.26	4.43	26,27,31,35	5
3	0NG	B	400	10/10	0.86	0.27	1.98	37,43,49,57	10
3	0NG	C	400	10/10	0.88	0.21	1.53	41,50,57,66	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	B	401	5/5	0.94	0.18	0.34	25,25,27,32	5
2	PO4	C	401	5/5	0.96	0.15	-0.19	26,27,27,30	5

6.5 Other polymers (i)

There are no such residues in this entry.