



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:28 AM GMT

PDB ID : 3AXX
Title : Functional analysis of hyperthermophilic endocellulase from the Archaeon Pyrococcus horikoshii
Authors : Kim, H.-W.; Ishikawa, K.
Deposited on : 2011-04-18
Resolution : 1.90 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

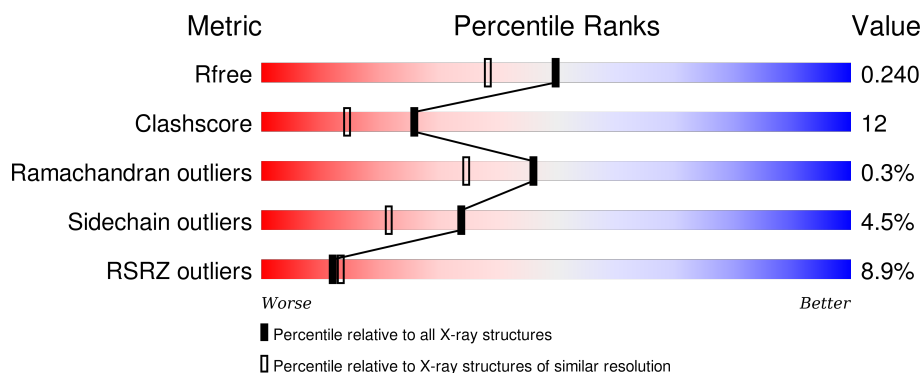
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 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 $\leq 5\%$. 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	458	<div> <div>7%</div> <div>67%</div> <div>15%</div> <div>•</div> <div>18%</div> </div>
1	B	458	<div> <div>6%</div> <div>64%</div> <div>17%</div> <div>•</div> <div>17%</div> </div>
1	C	458	<div> <div>9%</div> <div>56%</div> <div>24%</div> <div>•</div> <div>17%</div> </div>

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
3	PO4	A	461	-	-	-	X

2 Entry composition [i](#)

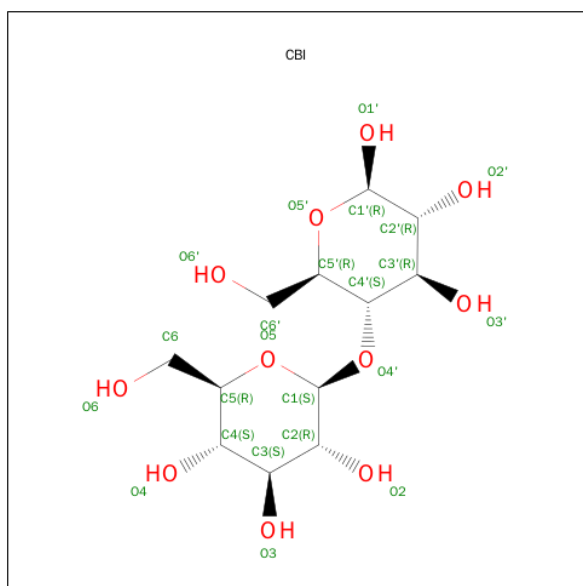
There are 4 unique types of molecules in this entry. The entry contains 9814 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 458aa long hypothetical endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3071	2002	502	557	10			
1	B	379	Total	C	N	O	S	0	0	0
			3090	2015	504	561	10			
1	C	378	Total	C	N	O	S	0	0	0
			3083	2011	503	559	10			

- Molecule 2 is SUGAR (CELLOBIOSE) (three-letter code: CBI) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

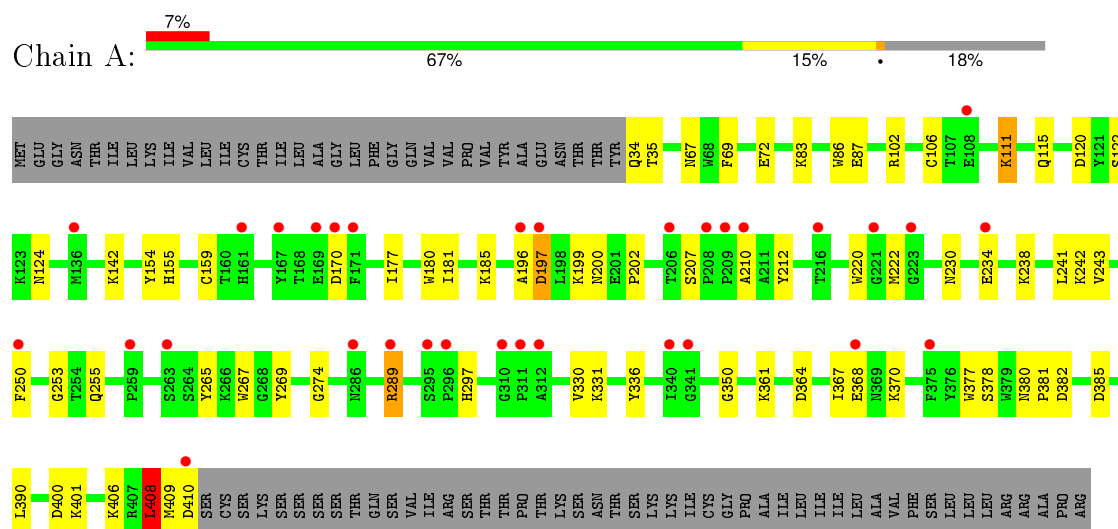
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	192	Total	O	0	0
			192	192		
4	B	189	Total	O	0	0
			189	189		
4	C	105	Total	O	0	0
			105	105		

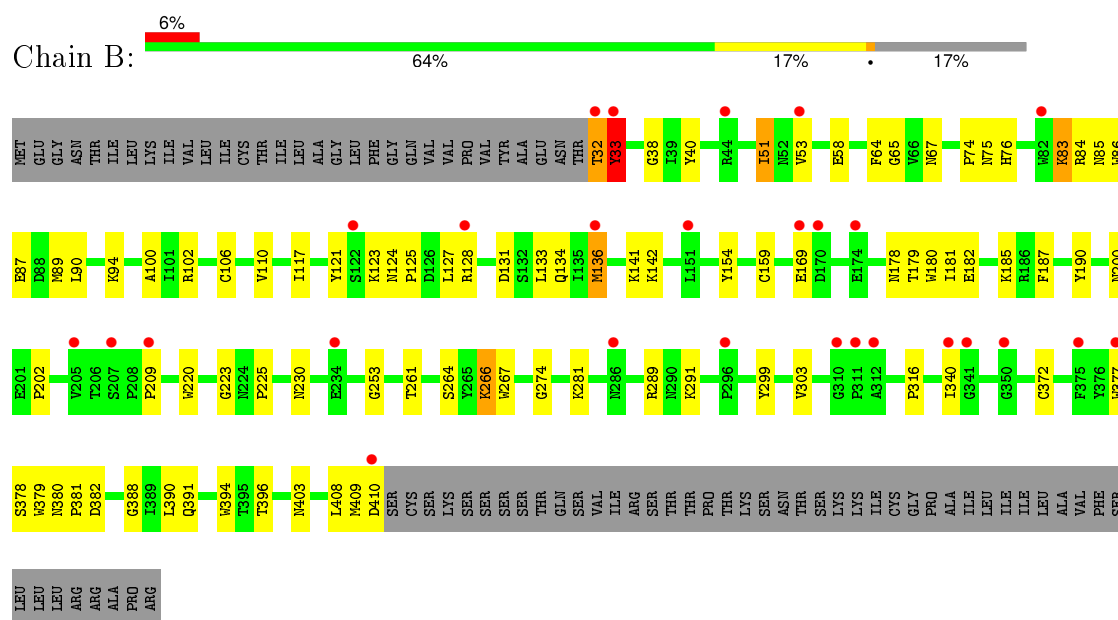
3 Residue-property plots [i](#)

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.

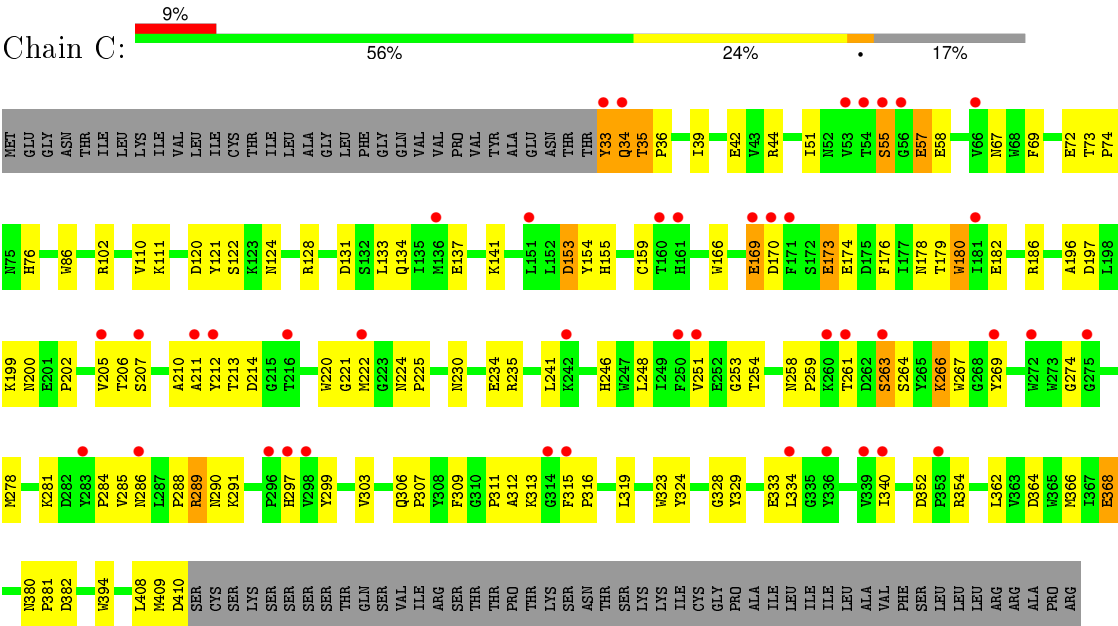
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.47Å 58.49Å 138.50Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 33.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-1.90) 94.7 (33.42-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.241 0.226 , 0.240	Depositor DCC
R_{free} test set	4609 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 91847 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9814	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, CBI

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	0.38	0/3182	0.69	2/4344 (0.0%)
1	B	0.40	1/3202 (0.0%)	0.71	2/4372 (0.0%)
1	C	0.36	0/3195	0.70	1/4362 (0.0%)
All	All	0.38	1/9579 (0.0%)	0.70	5/13078 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	ARG	CA-CB	-5.17	1.42	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	ARG	CB-CG-CD	-6.66	94.30	111.60
1	B	33	TYR	N-CA-C	5.86	126.82	111.00
1	A	408	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	197	ASP	N-CA-C	-5.16	97.08	111.00
1	C	197	ASP	N-CA-C	-5.16	97.08	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	3071	0	2910	54	0
1	B	3090	0	2926	71	0
1	C	3083	0	2919	98	0
2	A	23	0	22	0	0
2	B	23	0	22	0	0
2	C	23	0	22	1	0
3	A	15	0	0	0	0
4	A	192	0	0	10	1
4	B	189	0	0	8	0
4	C	105	0	0	2	0
All	All	9814	0	8821	223	1

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 12.

All (223) 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:266:LYS:HD2	1:C:266:LYS:H	1.15	1.10
1:A:212:TYR:HB3	1:A:222:MET:HE2	1.37	1.07
1:C:333:GLU:HG2	1:C:334:LEU:HD23	1.49	0.91
1:C:67:ASN:HD21	1:C:102:ARG:HH11	1.18	0.91
1:A:111:LYS:HZ2	1:A:111:LYS:HB3	1.34	0.91
1:B:372:CYS:HB2	4:B:483:HOH:O	1.75	0.85
1:B:51:ILE:HD13	1:B:58:GLU:HG2	1.60	0.84
1:A:212:TYR:HB3	1:A:222:MET:CE	2.08	0.83
1:A:111:LYS:HB3	1:A:111:LYS:NZ	1.92	0.82
1:B:83:LYS:O	1:B:83:LYS:HD3	1.80	0.80
1:B:86:TRP:HD1	1:B:124:ASN:HD22	1.27	0.79
1:B:106:CYS:HG	1:B:159:CYS:HG	1.27	0.79
1:C:289:ARG:O	1:C:289:ARG:HG3	1.83	0.78
1:C:67:ASN:ND2	1:C:102:ARG:HH11	1.81	0.77
1:C:289:ARG:O	1:C:289:ARG:CG	2.32	0.76
1:C:266:LYS:HD2	1:C:266:LYS:N	1.95	0.76
1:C:409:MET:O	1:C:410:ASP:HB2	1.86	0.75
1:C:35:THR:HB	1:C:246:HIS:HB3	1.68	0.73
1:B:110:VAL:HA	1:B:133:LEU:HD13	1.71	0.73
1:B:133:LEU:HG	4:B:642:HOH:O	1.87	0.73
1:A:67:ASN:HD21	1:A:102:ARG:HH11	1.35	0.72
1:B:33:TYR:H	1:B:33:TYR:HD1	1.35	0.71
1:C:169:GLU:HG3	1:C:170:ASP:N	2.05	0.71
1:B:136:MET:HE2	1:B:187:PHE:CZ	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:TYR:CD1	1:C:34:GLN:HG2	2.25	0.71
1:C:128:ARG:HD2	4:C:461:HOH:O	1.89	0.71
1:A:253:GLY:O	1:A:274:GLY:HA2	1.91	0.70
1:A:87:GLU:OE2	1:A:142:LYS:HE3	1.91	0.70
1:C:76:HIS:HE1	1:C:159:CYS:SG	2.13	0.70
1:B:67:ASN:HD21	1:B:102:ARG:HD3	1.57	0.69
1:A:106:CYS:HG	1:A:159:CYS:HG	0.69	0.69
1:B:340:ILE:HG13	4:B:486:HOH:O	1.93	0.69
1:A:120:ASP:OD1	1:A:122:SER:HB3	1.92	0.68
1:A:67:ASN:HD21	1:A:102:ARG:HD3	1.57	0.68
1:A:102:ARG:HH22	1:A:200:ASN:HD22	1.40	0.68
1:C:267:TRP:CZ3	1:C:307:PRO:HB2	2.28	0.68
1:B:134:GLN:HG3	4:B:636:HOH:O	1.92	0.67
1:A:86:TRP:HD1	1:A:124:ASN:HD22	1.43	0.67
1:B:67:ASN:HD21	1:B:102:ARG:HH11	1.42	0.67
1:A:86:TRP:H	1:A:124:ASN:HD21	1.41	0.65
1:C:33:TYR:HD1	1:C:34:GLN:HG2	1.59	0.65
1:A:234:GLU:HB2	4:A:640:HOH:O	1.95	0.65
1:C:333:GLU:HG2	1:C:334:LEU:CD2	2.26	0.65
1:B:84:ARG:NH1	1:B:394:TRP:O	2.29	0.63
1:C:186:ARG:HH11	1:C:186:ARG:HG3	1.64	0.63
1:C:86:TRP:H	1:C:124:ASN:HD21	1.46	0.62
1:B:391:GLN:HG3	1:B:396:THR:O	2.00	0.62
1:B:121:TYR:CD1	1:B:128:ARG:HG2	2.35	0.62
1:C:199:LYS:HD2	1:C:202:PRO:HG3	1.82	0.61
1:C:288:PRO:O	1:C:290:ASN:N	2.34	0.61
1:A:289:ARG:HB3	1:A:289:ARG:CZ	2.31	0.61
1:B:86:TRP:H	1:B:124:ASN:ND2	1.99	0.61
1:A:410:ASP:HB3	4:A:631:HOH:O	2.01	0.60
1:B:123:LYS:C	1:B:125:PRO:HD3	2.22	0.60
1:C:102:ARG:HH22	1:C:200:ASN:HD22	1.49	0.60
1:A:289:ARG:HG3	1:A:289:ARG:HH21	1.66	0.60
1:A:86:TRP:H	1:A:124:ASN:ND2	2.00	0.60
1:A:242:LYS:HE2	4:A:643:HOH:O	2.02	0.59
1:C:311:PRO:O	1:C:313:LYS:N	2.35	0.59
1:C:173:GLU:HG3	1:C:173:GLU:O	2.02	0.59
1:C:220:TRP:CE2	1:C:230:ASN:HB3	2.38	0.59
1:A:34:GLN:HA	4:A:472:HOH:O	2.02	0.59
1:A:67:ASN:ND2	1:A:102:ARG:HH11	2.01	0.59
1:C:364:ASP:O	1:C:368:GLU:HG3	2.03	0.59
1:B:131:ASP:OD1	1:B:134:GLN:CG	2.51	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:TRP:HD1	1:C:124:ASN:HD22	1.49	0.58
1:A:380:ASN:HB3	1:A:382:ASP:OD1	2.02	0.58
1:C:44:ARG:NH1	1:C:58:GLU:OE1	2.35	0.58
1:A:220:TRP:CE2	1:A:230:ASN:HB3	2.39	0.58
1:C:86:TRP:H	1:C:124:ASN:ND2	2.01	0.57
1:B:75:ASN:HA	1:B:117:ILE:HG12	1.86	0.57
1:C:35:THR:HG21	1:C:39:ILE:O	2.05	0.57
1:B:381:PRO:HD2	1:B:394:TRP:CZ2	2.39	0.57
1:B:409:MET:O	1:B:410:ASP:HB2	2.05	0.57
1:A:368:GLU:HG3	4:A:517:HOH:O	2.04	0.57
1:A:102:ARG:HH22	1:A:200:ASN:ND2	2.03	0.57
1:C:311:PRO:C	1:C:313:LYS:H	2.08	0.57
1:C:67:ASN:HD21	1:C:102:ARG:HD3	1.69	0.56
1:C:120:ASP:OD1	1:C:122:SER:HB3	2.06	0.56
1:B:266:LYS:HE2	1:B:267:TRP:NE1	2.19	0.56
1:B:253:GLY:O	1:B:274:GLY:HA2	2.06	0.56
1:C:35:THR:HB	1:C:246:HIS:CB	2.36	0.55
1:B:64:PHE:CD2	1:B:409:MET:HG2	2.41	0.55
1:C:34:GLN:C	1:C:35:THR:HG22	2.27	0.55
1:C:311:PRO:HA	1:C:315:PHE:HB3	1.88	0.55
1:A:385:ASP:HB3	4:A:647:HOH:O	2.05	0.55
1:B:67:ASN:ND2	1:B:102:ARG:HH11	2.04	0.55
1:A:367:ILE:HG13	1:A:408:LEU:HD13	1.89	0.55
1:B:124:ASN:N	1:B:125:PRO:HD3	2.21	0.55
1:B:209:PRO:HD2	4:B:632:HOH:O	2.07	0.54
1:B:86:TRP:H	1:B:124:ASN:HD21	1.55	0.54
1:C:186:ARG:HG3	1:C:186:ARG:NH1	2.21	0.54
1:B:32:THR:HA	1:B:40:TYR:CD2	2.42	0.54
1:B:86:TRP:HD1	1:B:124:ASN:ND2	2.00	0.53
1:C:253:GLY:O	1:C:274:GLY:HA2	2.07	0.53
1:C:329:TYR:O	1:C:333:GLU:HB3	2.08	0.53
1:A:207:SER:O	1:A:210:ALA:HB3	2.08	0.53
1:A:180:TRP:CH2	1:A:196:ALA:HB1	2.43	0.53
1:B:102:ARG:HH22	1:B:200:ASN:HD22	1.57	0.53
1:B:261:THR:O	1:B:264:SER:OG	2.20	0.53
1:C:131:ASP:OD1	1:C:134:GLN:HG3	2.09	0.53
1:C:281:LYS:O	1:C:284:PRO:HD3	2.09	0.53
1:C:222:MET:SD	1:C:259:PRO:HD3	2.49	0.52
1:C:267:TRP:HZ3	1:C:307:PRO:HB2	1.73	0.52
1:B:86:TRP:O	1:B:89:MET:HB2	2.10	0.52
1:C:33:TYR:HD1	1:C:34:GLN:N	2.07	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:THR:OG1	1:C:214:ASP:OD2	2.25	0.52
1:B:380:ASN:O	1:B:388:GLY:HA3	2.09	0.52
1:C:212:TYR:HB3	1:C:222:MET:HE1	1.92	0.51
1:B:141:LYS:HD2	4:B:476:HOH:O	2.10	0.51
1:C:340:ILE:HD12	1:C:366:MET:CE	2.40	0.51
1:B:136:MET:CE	1:B:187:PHE:CZ	2.94	0.51
1:B:379:TRP:CE2	1:B:390:LEU:HD11	2.46	0.50
1:B:181:ILE:O	1:B:185:LYS:HG3	2.12	0.50
1:C:352:ASP:OD1	1:C:354:ARG:HB2	2.11	0.50
1:B:86:TRP:N	1:B:124:ASN:HD21	2.09	0.50
1:A:289:ARG:CG	1:A:289:ARG:HH21	2.25	0.50
1:B:223:GLY:O	1:B:225:PRO:HD3	2.12	0.50
1:B:131:ASP:OD1	1:B:134:GLN:HG3	2.12	0.49
1:C:42:GLU:OE1	1:C:51:ILE:HD11	2.13	0.49
1:B:202:PRO:HD2	1:B:253:GLY:O	2.12	0.49
1:C:263:SER:HB3	1:C:269:TYR:OH	2.12	0.49
1:C:51:ILE:HG12	1:C:58:GLU:HB2	1.95	0.49
1:C:133:LEU:O	1:C:137:GLU:HG3	2.13	0.49
1:B:179:THR:O	1:B:182:GLU:HG3	2.13	0.49
1:C:258:ASN:ND2	1:C:261:THR:OG1	2.46	0.49
1:B:131:ASP:OD1	1:B:134:GLN:HG2	2.13	0.48
1:C:212:TYR:O	1:C:222:MET:HE2	2.13	0.48
1:C:334:LEU:N	1:C:334:LEU:HD23	2.27	0.48
1:C:206:THR:O	1:C:211:ALA:HB2	2.13	0.48
1:B:409:MET:O	1:B:410:ASP:CB	2.60	0.48
1:B:33:TYR:N	1:B:33:TYR:CD1	2.76	0.48
1:C:234:GLU:HG2	1:C:286:ASN:O	2.13	0.48
1:B:190:TYR:CD2	1:B:190:TYR:N	2.82	0.47
1:B:291:LYS:HA	1:B:291:LYS:HE2	1.95	0.47
1:B:220:TRP:CE2	1:B:230:ASN:HB3	2.49	0.47
1:A:86:TRP:N	1:A:124:ASN:HD21	2.11	0.47
1:B:178:ASN:O	1:B:182:GLU:HG2	2.14	0.47
1:A:381:PRO:HB3	1:A:390:LEU:O	2.14	0.47
1:B:299:TYR:CD1	1:B:303:VAL:HG21	2.49	0.47
1:C:299:TYR:CD1	1:C:303:VAL:HG21	2.49	0.47
1:B:85:ASN:HA	1:B:124:ASN:ND2	2.30	0.47
1:A:212:TYR:OH	1:A:269:TYR:HE1	1.98	0.47
1:C:324:TYR:HA	1:C:328:GLY:HA3	1.97	0.47
1:A:255:GLN:HB3	4:A:477:HOH:O	2.15	0.46
1:C:55:SER:HB2	1:C:57:GLU:HB2	1.97	0.46
1:A:409:MET:O	1:A:410:ASP:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:HG22	1:A:181:ILE:HD12	1.97	0.46
1:B:124:ASN:HB3	1:B:127:LEU:HD12	1.97	0.46
1:B:381:PRO:HD2	1:B:394:TRP:CH2	2.51	0.45
1:C:55:SER:C	1:C:57:GLU:H	2.18	0.45
1:C:380:ASN:HB3	1:C:382:ASP:OD1	2.16	0.45
1:B:87:GLU:CB	4:B:647:HOH:O	2.64	0.45
1:C:221:GLY:HA2	4:C:557:HOH:O	2.15	0.45
1:B:74:PRO:O	1:B:76:HIS:CD2	2.69	0.45
1:B:38:GLY:O	1:B:53:VAL:HG22	2.17	0.45
1:C:291:LYS:HE2	1:C:291:LYS:HA	1.98	0.45
1:B:74:PRO:HD3	1:B:159:CYS:O	2.17	0.45
1:C:200:ASN:ND2	1:C:297:HIS:HE1	2.15	0.45
1:C:306:GLN:HB2	1:C:309:PHE:CD2	2.52	0.45
1:B:83:LYS:C	1:B:83:LYS:HD3	2.29	0.45
1:A:330:VAL:HG12	1:A:336:TYR:HB2	1.98	0.44
1:A:265:TYR:CE2	1:A:267:TRP:HB2	2.52	0.44
1:A:370:LYS:HE2	4:A:544:HOH:O	2.18	0.44
1:C:137:GLU:OE2	1:C:186:ARG:NH1	2.51	0.44
1:B:380:ASN:HB3	1:B:382:ASP:OD1	2.18	0.44
1:C:235:ARG:HG3	1:C:235:ARG:HH11	1.82	0.44
1:C:409:MET:HE2	1:C:409:MET:HB2	1.71	0.43
1:C:368:GLU:C	1:C:368:GLU:OE2	2.56	0.43
1:C:306:GLN:NE2	2:C:459:CBI:O2'	2.47	0.43
1:A:331:LYS:HE3	1:A:370:LYS:O	2.18	0.43
1:C:311:PRO:C	1:C:313:LYS:N	2.72	0.43
1:C:288:PRO:O	1:C:289:ARG:C	2.57	0.43
1:A:367:ILE:HG13	1:A:408:LEU:CD1	2.48	0.43
1:C:281:LYS:NZ	1:C:281:LYS:HB3	2.33	0.43
1:C:278:MET:HA	1:C:329:TYR:OH	2.18	0.43
1:C:121:TYR:HB3	1:C:128:ARG:HD3	1.99	0.43
1:C:169:GLU:HG3	1:C:170:ASP:H	1.79	0.43
1:C:86:TRP:N	1:C:124:ASN:HD21	2.12	0.43
1:C:36:PRO:HD2	1:C:246:HIS:CE1	2.53	0.43
1:C:381:PRO:HD2	1:C:394:TRP:CH2	2.54	0.43
1:C:316:PRO:O	1:C:319:LEU:HG	2.19	0.43
1:C:102:ARG:HH22	1:C:200:ASN:ND2	2.15	0.43
1:C:224:ASN:HA	1:C:225:PRO:HD2	1.63	0.43
1:C:110:VAL:HA	1:C:133:LEU:HD13	1.99	0.43
1:B:90:LEU:HD12	1:B:142:LYS:CG	2.48	0.43
1:C:176:PHE:O	1:C:179:THR:HB	2.19	0.43
1:B:87:GLU:HB2	4:B:647:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:LEU:HD12	1:C:408:LEU:O	2.19	0.43
1:B:133:LEU:O	1:B:136:MET:HB2	2.20	0.42
1:C:166:TRP:CD1	1:C:173:GLU:HB2	2.54	0.42
1:A:200:ASN:ND2	1:A:297:HIS:HE1	2.17	0.42
1:B:121:TYR:CE1	1:B:128:ARG:HA	2.54	0.42
1:B:377:TRP:HA	1:B:378:SER:HA	1.79	0.42
1:B:67:ASN:ND2	1:B:102:ARG:HB3	2.34	0.42
1:C:261:THR:HG22	1:C:278:MET:HG3	2.01	0.42
1:A:361:LYS:HD2	4:A:615:HOH:O	2.20	0.42
1:B:64:PHE:CG	1:B:409:MET:HG2	2.55	0.41
1:B:65:GLY:HA2	1:B:100:ALA:O	2.21	0.41
1:C:241:LEU:HD23	1:C:241:LEU:HA	1.84	0.41
1:A:400:ASP:OD1	1:A:401:LYS:N	2.53	0.41
1:A:377:TRP:HA	1:A:378:SER:HA	1.75	0.41
1:B:281:LYS:HB3	1:B:281:LYS:HE2	1.95	0.41
1:C:178:ASN:O	1:C:182:GLU:HG3	2.20	0.41
1:B:85:ASN:HA	1:B:124:ASN:HD21	1.84	0.41
1:A:234:GLU:O	1:A:238:LYS:HG3	2.21	0.41
1:C:202:PRO:HB2	1:C:254:THR:HG22	2.02	0.41
1:A:364:ASP:O	1:A:368:GLU:HG3	2.21	0.41
1:A:406:LYS:HE3	1:A:406:LYS:HB2	1.82	0.41
1:C:153:ASP:C	1:C:153:ASP:OD1	2.58	0.41
1:A:197:ASP:HA	1:A:250:PHE:HB2	2.02	0.41
1:A:350:GLY:HA2	4:A:484:HOH:O	2.20	0.41
1:A:241:LEU:HA	1:A:241:LEU:HD23	1.93	0.41
1:C:324:TYR:CE2	1:C:329:TYR:HB3	2.55	0.40
1:A:199:LYS:CD	1:A:202:PRO:HG3	2.51	0.40
1:C:155:HIS:HA	1:C:200:ASN:HB3	2.02	0.40
1:C:69:PHE:HB2	1:C:72:GLU:OE2	2.21	0.40
1:C:251:VAL:HG11	1:C:285:VAL:HG21	2.03	0.40
1:C:180:TRP:CH2	1:C:196:ALA:HB1	2.57	0.40
1:C:73:THR:HB	1:C:74:PRO:CD	2.52	0.40
1:A:69:PHE:HB2	1:A:72:GLU:OE2	2.22	0.40
1:A:155:HIS:HA	1:A:200:ASN:HB3	2.03	0.40
1:C:323:TRP:CH2	1:C:362:LEU:HA	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:558:HOH:O	4:A:558:HOH:O[2_555]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	375/458 (82%)	364 (97%)	11 (3%)	0	100	100
1	B	377/458 (82%)	364 (97%)	13 (3%)	0	100	100
1	C	376/458 (82%)	337 (90%)	36 (10%)	3 (1%)	24	11
All	All	1128/1374 (82%)	1065 (94%)	60 (5%)	3 (0%)	46	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	312	ALA
1	C	289	ARG
1	C	210	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/396 (82%)	314 (97%)	10 (3%)	47	37
1	B	326/396 (82%)	313 (96%)	13 (4%)	38	26
1	C	325/396 (82%)	304 (94%)	21 (6%)	21	10
All	All	975/1188 (82%)	931 (96%)	44 (4%)	34	21

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	83	LYS
1	A	111	LYS
1	A	115	GLN
1	A	154	TYR
1	A	170	ASP
1	A	185	LYS
1	A	243	VAL
1	A	289	ARG
1	A	408	LEU
1	B	32	THR
1	B	33	TYR
1	B	51	ILE
1	B	83	LYS
1	B	94	LYS
1	B	136	MET
1	B	154	TYR
1	B	169	GLU
1	B	180	TRP
1	B	266	LYS
1	B	316	PRO
1	B	403	ASN
1	B	408	LEU
1	C	33	TYR
1	C	34	GLN
1	C	35	THR
1	C	55	SER
1	C	57	GLU
1	C	111	LYS
1	C	141	LYS
1	C	153	ASP
1	C	154	TYR
1	C	169	GLU
1	C	173	GLU
1	C	174	GLU
1	C	180	TRP
1	C	205	VAL
1	C	207	SER
1	C	213	THR
1	C	248	LEU
1	C	263	SER
1	C	264	SER
1	C	266	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	368	GLU

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	62	HIS
1	A	67	ASN
1	A	76	HIS
1	A	115	GLN
1	A	124	ASN
1	A	200	ASN
1	A	359	GLN
1	B	62	HIS
1	B	67	ASN
1	B	76	HIS
1	B	124	ASN
1	B	200	ASN
1	B	359	GLN
1	C	67	ASN
1	C	76	HIS
1	C	124	ASN
1	C	161	HIS
1	C	200	ASN
1	C	359	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 carbohydrates in this entry.

5.6 Ligand geometry

6 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	CBI	A	459	-	24,24,24	0.43	0	35,35,35	1.08	3 (8%)
3	PO4	A	460	-	4,4,4	1.15	0	6,6,6	0.27	0
3	PO4	A	461	-	4,4,4	1.11	0	6,6,6	0.27	0
3	PO4	A	462	-	4,4,4	1.14	0	6,6,6	0.27	0
2	CBI	B	459	-	24,24,24	0.42	0	35,35,35	1.10	2 (5%)
2	CBI	C	459	-	24,24,24	0.47	0	35,35,35	1.90	13 (37%)

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	CBI	A	459	-	-	0/8/48/48	0/2/2/2
3	PO4	A	460	-	-	0/0/0/0	0/0/0/0
3	PO4	A	461	-	-	0/0/0/0	0/0/0/0
3	PO4	A	462	-	-	0/0/0/0	0/0/0/0
2	CBI	B	459	-	-	0/8/48/48	0/2/2/2
2	CBI	C	459	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	459	CBI	O5'-C1'-C2'	-4.26	103.00	109.80
2	B	459	CBI	C1'-O5'-C5'	-3.49	107.01	113.47
2	C	459	CBI	C1-O4'-C4'	-3.23	109.56	118.01
2	C	459	CBI	C4-C3-C2	-3.09	105.02	110.79
2	C	459	CBI	O4'-C1-C2	-2.92	101.01	108.10
2	C	459	CBI	O5-C5-C6	-2.46	100.13	106.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	459	CBI	O6'-C6'-C5'	-2.41	103.37	111.33
2	C	459	CBI	O5-C1-C2	-2.32	105.52	110.28
2	A	459	CBI	C1'-O5'-C5'	-2.28	109.26	113.47
2	C	459	CBI	O5'-C5'-C6'	-2.25	100.67	106.36
2	C	459	CBI	O1'-C1'-O5'	-2.19	104.25	110.25
2	A	459	CBI	C6'-C5'-C4'	-2.01	107.38	113.25
2	C	459	CBI	O4-C4-C3	2.10	115.06	110.34
2	A	459	CBI	O5'-C5'-C6'	2.31	112.18	106.36
2	C	459	CBI	O5-C5-C4	2.33	114.05	109.68
2	B	459	CBI	O5'-C5'-C6'	2.53	112.76	106.36
2	C	459	CBI	C1'-C2'-C3'	2.94	114.80	110.43
2	C	459	CBI	C3'-C4'-C5'	3.31	118.33	110.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	459	CBI	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	377/458 (82%)	0.31	32 (8%) 13 15	16, 29, 49, 58	11 (2%)
1	B	379/458 (82%)	0.43	27 (7%) 19 21	16, 32, 56, 66	10 (2%)
1	C	378/458 (82%)	0.71	42 (11%) 7 8	23, 43, 62, 79	9 (2%)
All	All	1134/1374 (82%)	0.48	101 (8%) 12 13	16, 34, 58, 79	30 (2%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	TYR	11.1
1	B	33	TYR	8.1
1	C	136	MET	6.7
1	B	136	MET	6.4
1	B	32	THR	6.3
1	A	136	MET	6.0
1	B	311	PRO	5.3
1	C	34	GLN	5.0
1	B	286	ASN	4.3
1	A	170	ASP	4.3
1	C	53	VAL	4.2
1	C	55	SER	4.1
1	A	169	GLU	4.1
1	C	260	LYS	4.1
1	B	234	GLU	4.0
1	C	216	THR	3.9
1	C	205	VAL	3.8
1	A	234	GLU	3.7
1	B	122	SER	3.7
1	C	340	ILE	3.6
1	C	336	TYR	3.6
1	B	310	GLY	3.5
1	B	312	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	286	ASN	3.4
1	C	353	PRO	3.3
1	B	209	PRO	3.3
1	B	44	ARG	3.3
1	B	53	VAL	3.2
1	C	298	VAL	3.2
1	C	296	PRO	3.2
1	C	170	ASP	3.1
1	A	311	PRO	3.0
1	C	263	SER	3.0
1	C	160	THR	2.9
1	C	269	TYR	2.9
1	A	206	THR	2.9
1	C	54	THR	2.9
1	A	167	TYR	2.9
1	B	170	ASP	2.8
1	C	211	ALA	2.8
1	C	151	LEU	2.8
1	A	161	HIS	2.8
1	C	251	VAL	2.8
1	C	283	TYR	2.8
1	A	250	PHE	2.8
1	A	375	PHE	2.8
1	A	221	GLY	2.7
1	B	128	ARG	2.7
1	C	222	MET	2.7
1	B	350	GLY	2.7
1	B	340	ILE	2.7
1	C	161	HIS	2.7
1	A	312	ALA	2.6
1	C	314	GLY	2.6
1	C	297	HIS	2.6
1	C	339	VAL	2.6
1	B	410	ASP	2.6
1	A	410	ASP	2.6
1	A	171	PHE	2.6
1	B	82	TRP	2.5
1	B	341	GLY	2.5
1	C	334	LEU	2.5
1	C	66	VAL	2.5
1	B	174	GLU	2.5
1	C	169	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	223	GLY	2.4
1	B	296	PRO	2.4
1	B	151	LEU	2.4
1	C	272	TRP	2.3
1	C	212	TYR	2.3
1	A	340	ILE	2.3
1	B	377	TRP	2.3
1	A	296	PRO	2.3
1	A	210	ALA	2.3
1	C	275	GLY	2.3
1	C	171	PHE	2.3
1	C	286	ASN	2.3
1	A	310	GLY	2.3
1	A	368	GLU	2.3
1	A	259	PRO	2.3
1	A	108	GLU	2.3
1	A	208	PRO	2.2
1	B	375	PHE	2.2
1	A	295	SER	2.2
1	C	56	GLY	2.2
1	C	261	THR	2.2
1	B	205	VAL	2.2
1	A	196	ALA	2.2
1	C	207	SER	2.2
1	B	207	SER	2.2
1	A	209	PRO	2.1
1	B	169	GLU	2.1
1	A	341	GLY	2.1
1	A	263	SER	2.1
1	A	216	THR	2.1
1	C	250	PHE	2.1
1	A	289	ARG	2.0
1	C	181	ILE	2.0
1	C	315	PHE	2.0
1	A	197	ASP	2.0
1	C	242	LYS	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 [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	A	461	5/5	0.96	0.12	2.37	45,46,47,48	0
2	CBI	A	459	23/23	0.76	0.17	1.66	44,49,50,53	0
2	CBI	B	459	23/23	0.85	0.14	1.41	30,39,42,47	0
3	PO4	A	462	5/5	0.95	0.12	1.31	58,59,60,61	0
2	CBI	C	459	23/23	0.80	0.14	-0.34	51,53,54,57	0
3	PO4	A	460	5/5	0.98	0.08	-1.49	39,39,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.