Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 10:12 PM EDT

PDB ID	:	6P66
Title	:	The crystal structure of the XPB complex with Bax1 from Archaeoglobus fulgidus at 3.0 Angstrom resolution
Authors	:	DuPrez, K.T.; Fan, L.; Hilario, E.
Deposited on	:	2019-06-03
Resolution	:	3.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

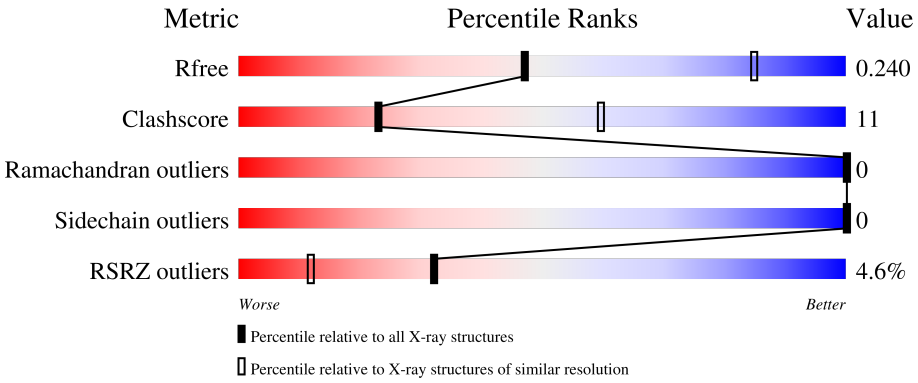
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	471	2% 71% 23% 6%
1	C	471	% 75% 23%
2	B	468	10% 84% 16%
2	D	468	6% 77% 23%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13249 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 DNA repair protein RAD25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3327	2138	582	602	5			
1	C	460	Total	C	N	O	S	0	0	0
			3430	2185	610	627	8			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP O29889
A	-17	GLY	-	expression tag	UNP O29889
A	-16	SER	-	expression tag	UNP O29889
A	-15	SER	-	expression tag	UNP O29889
A	-14	HIS	-	expression tag	UNP O29889
A	-13	HIS	-	expression tag	UNP O29889
A	-12	HIS	-	expression tag	UNP O29889
A	-11	HIS	-	expression tag	UNP O29889
A	-10	HIS	-	expression tag	UNP O29889
A	-9	SER	-	expression tag	UNP O29889
A	-8	SER	-	expression tag	UNP O29889
A	-7	GLY	-	expression tag	UNP O29889
A	-6	LEU	-	expression tag	UNP O29889
A	-5	VAL	-	expression tag	UNP O29889
A	-4	PRO	-	expression tag	UNP O29889
A	-3	ARG	-	expression tag	UNP O29889
A	-2	GLY	-	expression tag	UNP O29889
A	-1	SER	-	expression tag	UNP O29889
A	0	HIS	-	expression tag	UNP O29889
C	-18	MET	-	initiating methionine	UNP O29889
C	-17	GLY	-	expression tag	UNP O29889
C	-16	SER	-	expression tag	UNP O29889
C	-15	SER	-	expression tag	UNP O29889
C	-14	HIS	-	expression tag	UNP O29889
C	-13	HIS	-	expression tag	UNP O29889

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP O29889
C	-11	HIS	-	expression tag	UNP O29889
C	-10	HIS	-	expression tag	UNP O29889
C	-9	SER	-	expression tag	UNP O29889
C	-8	SER	-	expression tag	UNP O29889
C	-7	GLY	-	expression tag	UNP O29889
C	-6	LEU	-	expression tag	UNP O29889
C	-5	VAL	-	expression tag	UNP O29889
C	-4	PRO	-	expression tag	UNP O29889
C	-3	ARG	-	expression tag	UNP O29889
C	-2	GLY	-	expression tag	UNP O29889
C	-1	SER	-	expression tag	UNP O29889
C	0	HIS	-	expression tag	UNP O29889

- Molecule 2 is a protein called DNA endonuclease Bax1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	467	Total	C	N	O	S	0	0	0
			3058	1932	543	575	8			
2	D	467	Total	C	N	O	S	0	0	0
			3321	2123	578	610	10			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

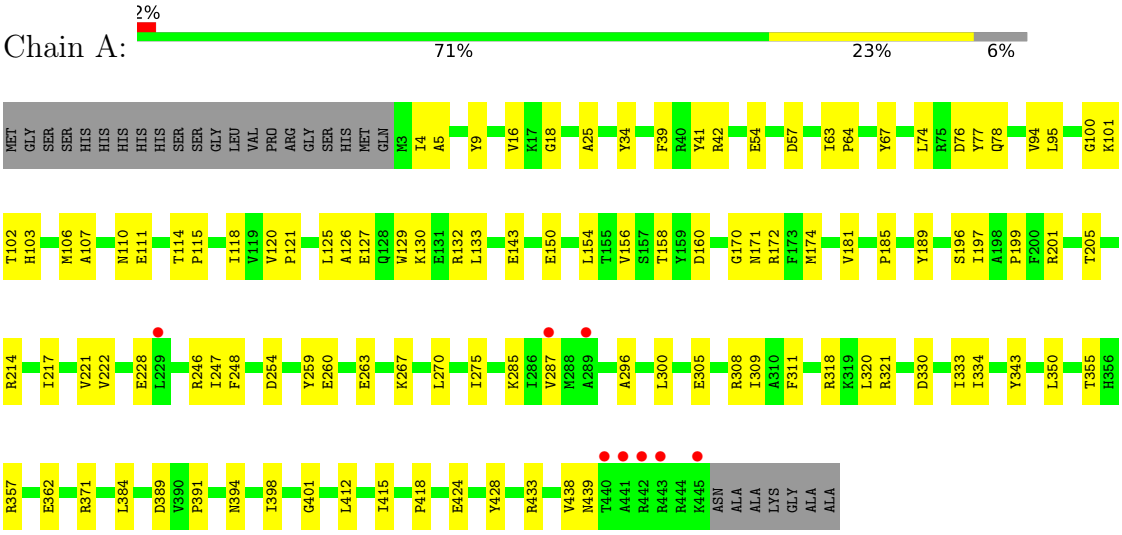
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	17	Total	O	0	0
			17	17		
4	C	32	Total	O	0	0
			32	32		
4	D	19	Total	O	0	0
			19	19		

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.

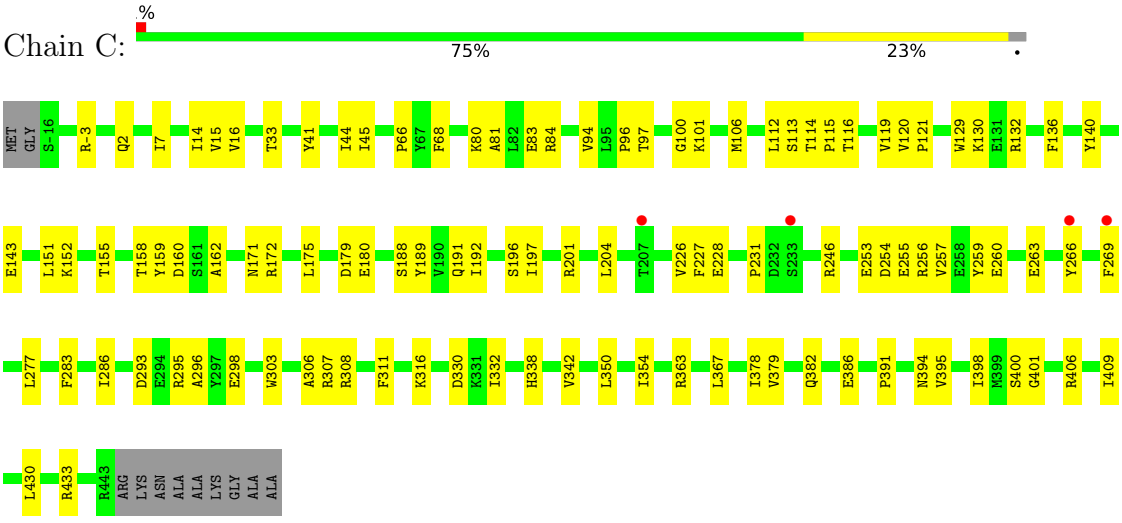
• Molecule 1: DNA repair protein RAD25

Chain A:



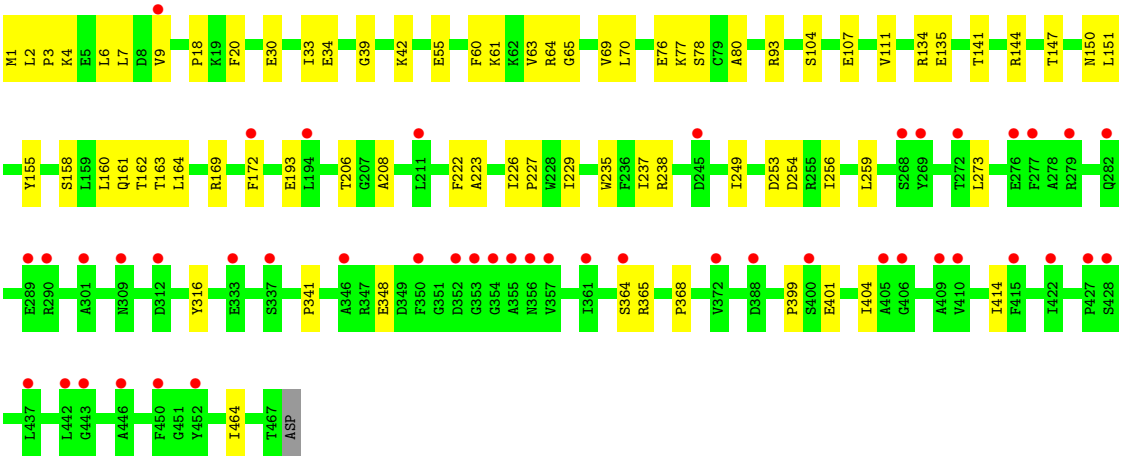
• Molecule 1: DNA repair protein RAD25

Chain C:

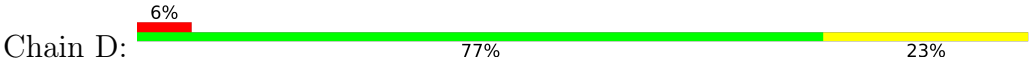


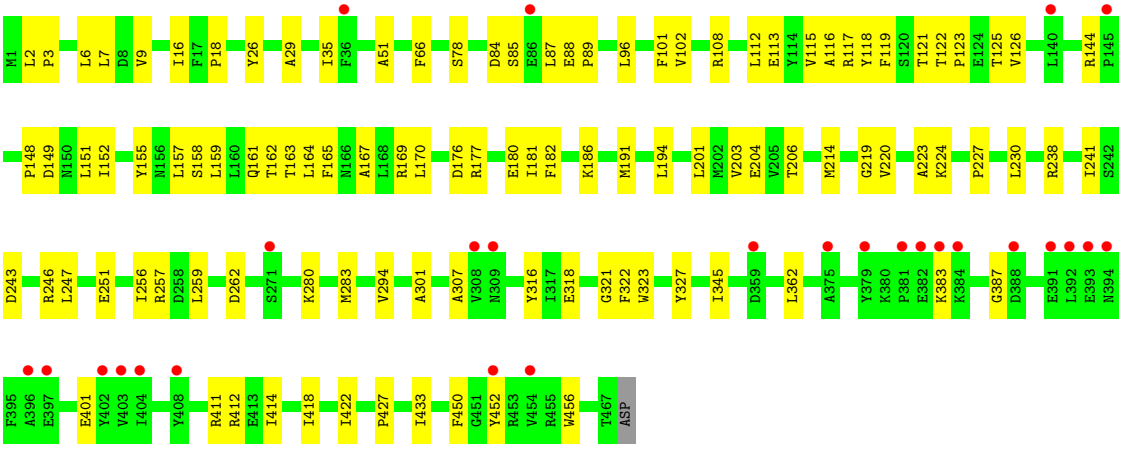
• Molecule 2: DNA endonuclease Bax1

Chain B:



• Molecule 2: DNA endonuclease Bax1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.60Å 129.84Å 108.15Å 90.00° 104.30° 90.00°	Depositor
Resolution (Å)	39.93 – 3.00 39.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.93-3.00) 98.3 (39.93-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.225 , 0.240 0.225 , 0.240	Depositor DCC
R_{free} test set	5288 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	97.9	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 104.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13249	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.36	0/3394	0.56	0/4604
1	C	0.32	0/3502	0.55	0/4758
2	B	0.31	0/3109	0.54	0/4261
2	D	0.30	0/3385	0.55	0/4607
All	All	0.32	0/13390	0.55	0/18230

There are no bond length outliers.

There are no bond angle outliers.

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	3327	0	3141	75	0
1	C	3430	0	3169	78	0
2	B	3058	0	2419	57	0
2	D	3321	0	2874	86	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
4	A	42	0	0	2	0
4	B	17	0	0	2	0
4	C	32	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	19	0	0	1	0
All	All	13249	0	11603	281	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 11.

All (281) 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)
2:D:87:LEU:HD11	2:D:119:PHE:CE2	1.80	1.17
2:B:464:ILE:HD13	2:D:433:ILE:HD11	1.43	0.98
1:A:67:TYR:HD1	1:A:433:ARG:NH2	1.64	0.94
1:A:67:TYR:HD1	1:A:433:ARG:HH22	1.06	0.91
2:D:122:THR:OG1	2:D:123:PRO:HD2	1.71	0.90
1:C:367:LEU:HD21	1:C:391:PRO:HG3	1.57	0.84
2:D:87:LEU:HD11	2:D:119:PHE:HE2	1.33	0.84
2:D:122:THR:OG1	2:D:123:PRO:CD	2.25	0.84
1:C:14:ILE:HD11	1:C:44:ILE:HD12	1.61	0.82
2:D:18:PRO:HB3	2:D:159:LEU:HD22	1.60	0.82
1:A:270:LEU:HB2	1:A:275:ILE:HD11	1.62	0.81
2:D:122:THR:HG23	2:D:125:THR:H	1.45	0.81
1:C:116:THR:HG22	1:C:175:LEU:HB3	1.64	0.80
1:C:132:ARG:HH21	1:C:132:ARG:HG2	1.47	0.78
1:C:308:ARG:HD2	4:C:602:HOH:O	1.84	0.77
1:A:67:TYR:CD1	1:A:433:ARG:NH2	2.52	0.76
1:A:267:LYS:HD2	1:A:270:LEU:HD11	1.67	0.76
1:C:311:PHE:HD2	1:C:338:HIS:HB2	1.50	0.75
1:A:181:VAL:HG12	1:A:205:THR:HB	1.68	0.73
1:C:342:VAL:HG23	1:C:379:VAL:HG22	1.71	0.72
2:D:87:LEU:HD11	2:D:119:PHE:CD2	2.23	0.72
1:A:320:LEU:HD21	1:A:334:ILE:HD13	1.71	0.72
2:B:161:GLN:HB2	2:B:223:ALA:HB1	1.73	0.70
2:D:113:GLU:O	2:D:117:ARG:HG3	1.92	0.70
2:D:123:PRO:HA	2:D:126:VAL:HG12	1.74	0.69
1:A:247:ILE:HD11	1:A:428:TYR:HD1	1.57	0.69
2:B:414:ILE:CB	4:B:508:HOH:O	2.40	0.69
2:D:123:PRO:O	2:D:126:VAL:HG12	1.92	0.69
2:D:256:ILE:HB	2:D:259:LEU:HD12	1.75	0.68
1:C:311:PHE:CD2	1:C:338:HIS:HB2	2.28	0.68
2:D:194:LEU:HB3	2:D:301:ALA:HB3	1.77	0.67
2:D:257:ARG:HH12	2:D:262:ASP:HB2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:SER:OG	2:B:107:GLU:HG2	1.95	0.66
2:B:2:LEU:H	2:B:162:THR:HG21	1.60	0.66
2:D:102:VAL:HG11	2:D:108:ARG:HB2	1.79	0.65
1:A:94:VAL:HG22	1:A:228:GLU:HA	1.79	0.65
2:B:144:ARG:HD3	4:B:507:HOH:O	1.97	0.64
1:A:247:ILE:HD12	1:A:247:ILE:N	2.12	0.64
2:D:87:LEU:CD1	2:D:119:PHE:CE2	2.72	0.64
2:D:411:ARG:O	2:D:414:ILE:HG13	1.98	0.63
1:C:132:ARG:HG2	1:C:132:ARG:NH2	2.12	0.63
1:C:398:ILE:HD12	1:C:409:ILE:HD13	1.80	0.63
1:A:94:VAL:HG12	1:A:205:THR:HG23	1.82	0.62
1:A:260:GLU:HA	1:A:263:GLU:HB3	1.80	0.62
2:B:235:TRP:H	2:B:254:ASP:HB3	1.65	0.62
1:A:102:THR:O	1:A:106:MET:HG2	1.99	0.62
2:D:280:LYS:HA	2:D:283:MET:HG2	1.80	0.62
2:B:6:LEU:HD11	2:B:64:ARG:HB3	1.82	0.61
2:D:2:LEU:HB3	2:D:162:THR:HG21	1.82	0.61
1:C:277:LEU:HD13	1:C:286:ILE:HD13	1.82	0.61
2:B:33:ILE:HD11	2:B:151:LEU:HD22	1.82	0.61
1:A:41:TYR:OH	1:A:57:ASP:OD2	2.19	0.61
2:B:172:PHE:HB2	2:B:237:ILE:HG12	1.83	0.61
1:C:-3:ARG:HB2	1:C:2:GLN:HB2	1.83	0.60
1:C:120:VAL:O	1:C:158:THR:HA	2.00	0.60
1:C:120:VAL:HG11	1:C:129:TRP:CD1	2.36	0.59
1:C:97:THR:HG23	1:C:100:GLY:H	1.67	0.59
1:C:119:VAL:HG12	1:C:159:TYR:CD1	2.37	0.59
2:D:246:ARG:NH2	2:D:247:LEU:O	2.36	0.59
2:D:194:LEU:HG	2:D:203:VAL:HG12	1.84	0.58
2:B:30:GLU:O	2:B:34:GLU:HG2	2.03	0.58
1:C:263:GLU:HA	1:C:266:TYR:CD1	2.38	0.58
1:A:333:ILE:HD12	1:A:415:ILE:HD13	1.86	0.58
2:B:365:ARG:H	2:B:368:PRO:HB3	1.69	0.58
1:C:130:LYS:NZ	1:C:143:GLU:HB2	2.19	0.58
2:D:230:LEU:O	2:D:257:ARG:NE	2.30	0.58
1:A:114:THR:HB	1:A:174:MET:HB2	1.86	0.57
1:C:171:ASN:HA	1:C:197:ILE:HG12	1.85	0.57
1:A:362:GLU:OE2	2:B:93:ARG:HD2	2.05	0.57
2:D:29:ALA:HB1	2:D:151:LEU:HD23	1.85	0.57
1:A:95:LEU:HD12	1:A:101:LYS:HA	1.86	0.56
1:C:332:ILE:HD12	2:D:101:PHE:CZ	2.39	0.56
1:C:386:GLU:HB2	2:D:214:MET:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TYR:CE1	1:A:78:GLN:HG3	2.40	0.56
1:C:84:ARG:HG2	1:C:226:VAL:HG22	1.86	0.56
1:A:384:LEU:HD11	1:A:412:LEU:HB2	1.86	0.56
2:B:158:SER:HA	2:B:161:GLN:HG2	1.87	0.56
2:D:414:ILE:O	2:D:418:ILE:HG12	2.06	0.56
2:D:433:ILE:HD12	2:D:433:ILE:H	1.70	0.56
2:B:256:ILE:HG23	2:B:259:LEU:HD12	1.88	0.55
1:A:74:LEU:HD11	1:A:107:ALA:HB2	1.88	0.55
1:A:267:LYS:HD3	1:A:270:LEU:HD21	1.87	0.55
1:A:308:ARG:HA	1:A:311:PHE:CD1	2.42	0.55
1:A:287:VAL:HG23	1:A:296:ALA:HB1	1.89	0.55
2:D:345:ILE:HG22	2:D:362:LEU:HB2	1.88	0.55
2:D:149:ASP:HA	2:D:152:ILE:HG12	1.89	0.55
2:B:158:SER:O	2:B:162:THR:HG23	2.07	0.55
1:A:133:LEU:HD22	1:A:154:LEU:HD23	1.88	0.54
2:B:55:GLU:OE2	2:B:64:ARG:HD2	2.06	0.54
2:D:158:SER:O	2:D:162:THR:HG23	2.07	0.54
1:C:188:SER:O	1:C:191:GLN:HG3	2.08	0.54
1:C:162:ALA:O	1:C:192:ILE:HG12	2.07	0.54
1:A:5:ALA:HA	1:A:18:GLY:HA3	1.89	0.54
1:C:130:LYS:HZ3	1:C:143:GLU:HB2	1.73	0.54
1:C:15:VAL:HG13	1:C:33:THR:HB	1.89	0.54
2:D:164:LEU:HD22	2:D:170:LEU:HD12	1.90	0.54
1:A:398:ILE:HG22	1:A:401:GLY:H	1.72	0.54
2:D:169:ARG:HD2	2:D:204:GLU:OE2	2.08	0.54
1:A:64:PRO:HB3	1:A:439:ASN:HB3	1.89	0.53
1:A:120:VAL:O	1:A:158:THR:HA	2.08	0.53
1:A:357:ARG:HH12	2:B:134:ARG:HE	1.57	0.53
1:A:259:TYR:O	1:A:263:GLU:N	2.39	0.53
1:C:332:ILE:HG12	1:C:395:VAL:CG1	2.38	0.53
1:A:275:ILE:O	1:A:275:ILE:HD12	2.08	0.53
1:C:171:ASN:OD1	1:C:172:ARG:HG3	2.09	0.53
1:C:293:ASP:HB3	1:C:296:ALA:HB2	1.90	0.52
2:D:87:LEU:CD1	2:D:119:PHE:CD2	2.92	0.52
2:D:157:LEU:HD21	2:D:227:PRO:HG3	1.91	0.52
2:D:422:ILE:HD12	2:D:450:PHE:CD2	2.45	0.52
1:A:418:PRO:HG3	1:A:424:GLU:HA	1.92	0.52
1:C:332:ILE:HD12	2:D:101:PHE:HZ	1.75	0.52
2:B:316:TYR:H	2:B:341:PRO:HG2	1.75	0.52
1:A:350:LEU:CD1	2:B:111:VAL:HG11	2.40	0.52
1:A:25:ALA:HB1	1:A:34:TYR:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:THR:O	2:B:150:ASN:N	2.43	0.51
2:B:160:LEU:O	2:B:163:THR:OG1	2.25	0.51
2:D:9:VAL:HG21	2:D:16:ILE:HD11	1.92	0.51
1:C:266:TYR:CE2	1:C:303:TRP:HD1	2.28	0.51
1:C:152:LYS:H	1:C:155:THR:CG2	2.23	0.51
1:C:386:GLU:HB2	2:D:214:MET:HA	1.92	0.51
2:B:399:PRO:HD2	2:D:412:ARG:HB2	1.92	0.51
1:C:80:LYS:N	1:C:406:ARG:HH12	2.09	0.51
1:C:151:LEU:HD13	1:C:172:ARG:HE	1.76	0.51
1:C:316:LYS:HE2	1:C:400:SER:O	2.11	0.51
1:A:42:ARG:HG2	1:A:199:PRO:HB3	1.92	0.50
2:B:33:ILE:HD13	2:B:70:LEU:HD22	1.94	0.50
1:C:254:ASP:O	1:C:257:VAL:HG22	2.11	0.50
1:A:103:HIS:CE1	4:A:602:HOH:O	2.65	0.50
1:A:196:SER:O	1:A:201:ARG:NH2	2.44	0.50
1:C:311:PHE:HD2	1:C:338:HIS:CB	2.22	0.50
1:A:287:VAL:HG11	1:A:300:LEU:HD22	1.94	0.50
1:C:41:TYR:CZ	1:C:45:ILE:HD11	2.46	0.50
1:C:433:ARG:HG3	4:C:618:HOH:O	2.11	0.50
1:C:350:LEU:HD22	2:D:96:LEU:HB3	1.93	0.49
1:A:143:GLU:O	1:A:150:GLU:HG2	2.13	0.49
2:D:238:ARG:NH2	2:D:251:GLU:OE2	2.38	0.49
1:C:269:PHE:CD1	1:C:295:ARG:HG3	2.48	0.49
2:B:80:ALA:O	2:B:141:THR:OG1	2.20	0.49
2:B:193:GLU:O	2:B:206:THR:HG22	2.13	0.49
2:B:76:GLU:HG2	2:B:77:LYS:HE3	1.93	0.49
1:C:112:LEU:HD12	1:C:175:LEU:HD22	1.95	0.49
1:C:307:ARG:NH1	4:C:601:HOH:O	2.38	0.49
2:D:191:MET:HB2	2:D:206:THR:HB	1.95	0.49
1:A:318:ARG:HG2	1:A:321:ARG:NH2	2.28	0.49
1:C:101:LYS:HD2	1:C:204:LEU:HB3	1.95	0.49
1:C:132:ARG:NH2	1:C:132:ARG:CG	2.72	0.49
2:B:464:ILE:HD12	2:D:452:TYR:CD1	2.48	0.48
2:D:115:VAL:HG13	2:D:126:VAL:HG21	1.95	0.48
2:B:2:LEU:HD12	2:B:3:PRO:HD2	1.94	0.48
2:D:84:ASP:OD1	2:D:85:SER:N	2.45	0.48
1:A:110:ASN:ND2	1:A:248:PHE:HE2	2.10	0.48
2:D:186:LYS:NZ	2:D:318:GLU:OE1	2.32	0.48
2:D:294:VAL:HG11	2:D:316:TYR:HE1	1.77	0.48
1:A:67:TYR:CE2	1:A:438:VAL:HB	2.48	0.48
1:C:311:PHE:CD1	1:C:401:GLY:HA3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ASP:OD1	1:A:389:ASP:N	2.35	0.47
2:D:116:ALA:HB1	2:D:121:THR:O	2.14	0.47
1:C:114:THR:OG1	1:C:115:PRO:HD2	2.13	0.47
2:D:123:PRO:CA	2:D:126:VAL:HG12	2.40	0.47
1:C:121:PRO:HG2	1:C:180:GLU:HG3	1.95	0.47
2:D:7:LEU:HD11	2:D:163:THR:CG2	2.44	0.47
1:A:121:PRO:HD2	1:A:125:LEU:HD12	1.97	0.47
1:C:7:ILE:HG22	1:C:16:VAL:HG22	1.95	0.47
2:D:123:PRO:O	2:D:126:VAL:CG1	2.62	0.47
2:D:3:PRO:HD2	2:D:6:LEU:HD21	1.95	0.47
2:B:226:ILE:HD12	2:B:229:ILE:HD12	1.97	0.47
1:A:102:THR:O	1:A:106:MET:N	2.43	0.47
2:B:2:LEU:H	2:B:162:THR:CG2	2.27	0.47
2:B:18:PRO:HG2	2:B:20:PHE:CE2	2.50	0.47
2:D:118:TYR:O	2:D:118:TYR:CD2	2.68	0.47
2:B:60:PHE:HA	2:B:63:VAL:HG12	1.96	0.47
2:B:401:GLU:O	2:B:404:ILE:HD11	2.16	0.46
1:C:354:ILE:HD11	1:C:378:ILE:HD11	1.96	0.46
1:A:4:ILE:HD11	1:A:54:GLU:HG3	1.97	0.46
1:C:260:GLU:HA	1:C:263:GLU:HG2	1.98	0.46
2:D:87:LEU:CD1	2:D:119:PHE:HE2	2.16	0.46
1:C:96:PRO:HB3	1:C:231:PRO:HA	1.97	0.46
1:A:160:ASP:OD1	1:A:189:TYR:OH	2.23	0.46
1:C:283:PHE:HA	1:C:286:ILE:HG12	1.97	0.46
1:A:171:ASN:HA	1:A:197:ILE:HG12	1.98	0.46
1:A:371:ARG:HE	1:A:391:PRO:HG3	1.81	0.46
2:D:88:GLU:HA	2:D:89:PRO:HD3	1.81	0.46
1:A:120:VAL:HG11	1:A:129:TRP:CD1	2.51	0.45
1:C:66:PRO:HG3	1:C:140:TYR:CE1	2.50	0.45
2:B:348:GLU:CB	2:B:364:SER:H	2.29	0.45
1:C:160:ASP:OD1	1:C:189:TYR:OH	2.29	0.45
1:A:185:PRO:HB2	1:A:214:ARG:NH1	2.31	0.45
2:D:155:TYR:CZ	2:D:159:LEU:HD12	2.50	0.45
2:D:161:GLN:HB3	2:D:223:ALA:HB1	1.98	0.45
2:B:7:LEU:HG	2:B:9:VAL:HG23	1.98	0.45
1:A:285:LYS:HE3	2:B:4:LYS:O	2.16	0.45
1:C:7:ILE:HA	1:C:15:VAL:O	2.17	0.45
2:D:176:ASP:CG	2:D:177:ARG:HG3	2.37	0.45
1:A:76:ASP:OD1	1:A:77:TYR:N	2.47	0.45
2:B:55:GLU:HA	2:B:63:VAL:HG11	1.99	0.45
2:B:226:ILE:HG22	2:B:227:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:TRP:CE2	2:B:254:ASP:HA	2.52	0.45
1:A:100:GLY:HA3	4:A:609:HOH:O	2.16	0.44
2:B:238:ARG:NH2	2:B:249:ILE:HD13	2.31	0.44
1:C:259:TYR:CE1	1:C:306:ALA:HB1	2.52	0.44
2:D:6:LEU:HD23	2:D:6:LEU:H	1.82	0.44
2:D:35:ILE:HD13	2:D:51:ALA:HA	1.99	0.44
2:D:294:VAL:HG21	2:D:307:ALA:CB	2.47	0.44
1:A:114:THR:HB	1:A:115:PRO:HD2	2.00	0.44
2:B:2:LEU:N	2:B:162:THR:HG21	2.27	0.44
2:B:273:LEU:HD23	2:B:273:LEU:O	2.17	0.44
1:A:106:MET:HE2	1:A:132:ARG:HB3	1.98	0.44
2:B:1:MET:HE3	2:B:69:VAL:HG22	2.00	0.44
2:D:194:LEU:CB	2:D:301:ALA:HB3	2.46	0.44
1:C:101:LYS:NZ	1:C:179:ASP:OD1	2.39	0.44
2:D:26:TYR:CD1	2:D:148:PRO:HB2	2.52	0.44
2:B:6:LEU:HA	2:B:61:LYS:HZ2	1.82	0.44
1:C:114:THR:O	1:C:116:THR:HG23	2.17	0.44
1:A:9:TYR:OH	1:A:170:GLY:HA3	2.18	0.43
1:A:127:GLU:HA	1:A:130:LYS:HG2	2.00	0.43
2:D:108:ARG:NH2	2:D:112:LEU:HD11	2.33	0.43
2:D:167:ALA:HA	2:D:241:ILE:HG22	2.00	0.43
1:C:196:SER:O	1:C:201:ARG:NH2	2.51	0.43
2:D:165:PHE:CE1	2:D:219:GLY:HA3	2.53	0.43
2:D:66:PHE:CZ	2:D:152:ILE:HG22	2.53	0.43
1:A:305:GLU:O	1:A:309:ILE:HG12	2.18	0.43
2:B:78:SER:HA	2:B:144:ARG:HH21	1.84	0.43
2:D:427:PRO:HG3	2:D:433:ILE:HG13	2.00	0.43
1:A:111:GLU:OE1	1:A:246:ARG:NH1	2.51	0.43
1:C:94:VAL:CG2	1:C:228:GLU:HA	2.48	0.43
2:B:164:LEU:HB3	2:B:222:PHE:HE2	1.83	0.43
1:C:121:PRO:CG	1:C:180:GLU:HG3	2.49	0.43
1:C:120:VAL:HG12	1:C:179:ASP:HB3	2.01	0.43
2:D:177:ARG:O	2:D:181:ILE:HG12	2.19	0.43
2:B:65:GLY:HA3	2:B:155:TYR:HE1	1.84	0.43
1:C:311:PHE:CE1	1:C:401:GLY:HA3	2.54	0.43
2:D:177:ARG:NH2	2:D:180:GLU:OE1	2.52	0.43
1:A:217:ILE:O	1:A:221:VAL:HG22	2.19	0.42
2:B:169:ARG:HA	2:B:208:ALA:HA	2.01	0.42
1:C:295:ARG:HA	1:C:298:GLU:HG2	2.00	0.42
2:D:243:ASP:O	2:D:246:ARG:HB3	2.19	0.42
1:A:63:ILE:HG12	1:A:172:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ILE:CD1	1:C:378:ILE:HD11	2.48	0.42
2:D:321:GLY:O	2:D:323:TRP:HD1	2.02	0.42
1:C:316:LYS:HZ1	1:C:430:LEU:C	2.22	0.42
1:C:330:ASP:HB3	1:C:394:ASN:OD1	2.19	0.42
1:A:214:ARG:O	1:A:217:ILE:HG22	2.19	0.42
1:C:263:GLU:HA	1:C:266:TYR:HD1	1.84	0.42
1:C:363:ARG:NH2	1:C:382:GLN:OE1	2.52	0.42
2:D:7:LEU:HD11	2:D:163:THR:HG23	2.01	0.42
1:C:106:MET:O	1:C:136:PHE:HZ	2.02	0.42
1:A:357:ARG:NH1	2:B:134:ARG:HE	2.18	0.42
2:B:39:GLY:O	2:B:42:LYS:HB2	2.19	0.42
2:D:78:SER:CB	2:D:144:ARG:HB2	2.50	0.42
1:A:16:VAL:HG13	1:A:34:TYR:HB2	2.01	0.42
1:A:39:PHE:HB2	1:A:201:ARG:HH12	1.84	0.42
2:B:226:ILE:HA	2:B:229:ILE:HD12	2.02	0.42
1:C:254:ASP:OD1	1:C:255:GLU:N	2.53	0.42
2:D:294:VAL:HG11	2:D:316:TYR:CE1	2.55	0.42
1:A:247:ILE:HD11	1:A:428:TYR:CD1	2.47	0.41
1:C:68:PHE:CD2	1:C:113:SER:HA	2.55	0.41
1:C:81:ALA:HB2	1:C:227:PHE:CD2	2.54	0.41
1:A:343:TYR:CE2	1:A:355:THR:HG21	2.55	0.41
2:D:191:MET:HB3	2:D:327:TYR:CE1	2.54	0.41
2:D:220:VAL:O	2:D:224:LYS:HG2	2.21	0.41
2:D:383:LYS:HA	2:D:387:GLY:CA	2.50	0.41
1:A:118:ILE:HD13	1:A:133:LEU:HD11	2.03	0.41
1:A:330:ASP:HB3	1:A:394:ASN:HB2	2.03	0.41
2:B:401:GLU:CB	2:D:401:GLU:CB	2.98	0.41
2:D:155:TYR:CE2	2:D:159:LEU:HD12	2.55	0.41
2:D:294:VAL:HG21	2:D:307:ALA:HB3	2.02	0.41
1:A:201:ARG:HB3	1:A:222:VAL:HG23	2.02	0.41
1:A:357:ARG:HH21	2:B:135:GLU:HG3	1.85	0.41
1:C:83:GLU:HG2	1:C:246:ARG:HH22	1.86	0.41
2:D:322:PHE:N	2:D:322:PHE:CD1	2.89	0.40
2:B:256:ILE:O	2:B:256:ILE:HG22	2.20	0.40
2:D:115:VAL:CG1	2:D:126:VAL:HG21	2.51	0.40
2:D:123:PRO:HA	2:D:126:VAL:CG1	2.49	0.40
2:D:182:PHE:HZ	2:D:201:LEU:HD21	1.85	0.40
2:B:365:ARG:N	2:B:368:PRO:HB3	2.36	0.40
1:A:126:ALA:HA	1:A:156:VAL:HG11	2.04	0.40
1:A:254:ASP:N	1:A:254:ASP:OD1	2.54	0.40
2:B:253:ASP:H	2:B:256:ILE:HD13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:GLU:O	1:C:257:VAL:HG13	2.21	0.40
1:C:256:ARG:O	1:C:260:GLU:HG2	2.21	0.40
2:D:456:TRP:HB2	4:D:509:HOH:O	2.20	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	441/471 (94%)	421 (96%)	20 (4%)	0	100	100
1	C	458/471 (97%)	434 (95%)	24 (5%)	0	100	100
2	B	465/468 (99%)	433 (93%)	32 (7%)	0	100	100
2	D	465/468 (99%)	437 (94%)	28 (6%)	0	100	100
All	All	1829/1878 (97%)	1725 (94%)	104 (6%)	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	302/397 (76%)	302 (100%)	0	100	100
1	C	309/397 (78%)	309 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/411 (49%)	202 (100%)	0	100	100
2	D	263/411 (64%)	263 (100%)	0	100	100
All	All	1076/1616 (67%)	1076 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	443/471 (94%)	-0.19	8 (1%) 68 40	58, 90, 160, 214	0
1	C	460/471 (97%)	-0.17	4 (0%) 84 63	58, 95, 163, 210	0
2	B	467/468 (99%)	0.33	46 (9%) 7 2	66, 156, 233, 260	0
2	D	467/468 (99%)	0.04	27 (5%) 23 7	67, 122, 200, 244	0
All	All	1837/1878 (97%)	0.01	85 (4%) 32 12	58, 109, 214, 260	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	443	GLY	7.7
2	B	277	PHE	7.2
2	B	409	ALA	6.7
2	D	391	GLU	5.7
2	B	353	GLY	5.5
2	B	352	ASP	5.4
2	B	354	GLY	5.3
2	B	290	ARG	5.2
2	B	268	SER	5.0
1	A	441	ALA	4.8
2	B	355	ALA	4.7
2	B	450	PHE	4.7
2	B	301	ALA	4.4
1	A	440	THR	4.4
2	B	428	SER	4.3
2	B	289	GLU	3.9
2	B	346	ALA	3.9
2	D	402	TYR	3.7
2	D	394	ASN	3.6
1	A	442	ARG	3.6
2	B	276	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	361	ILE	3.4
2	D	308	VAL	3.4
2	B	350	PHE	3.4
2	D	381	PRO	3.3
1	A	443	ARG	3.2
2	D	396	ALA	3.2
2	D	392	LEU	3.2
2	D	393	GLU	3.2
2	B	172	PHE	3.1
2	B	405	ALA	3.1
2	B	406	GLY	3.1
2	B	388	ASP	3.0
1	C	207	THR	3.0
2	B	269	TYR	3.0
2	D	271	SER	2.9
2	B	410	VAL	2.9
2	B	357	VAL	2.9
2	D	86	GLU	2.8
2	B	422	ILE	2.8
2	B	427	PRO	2.8
2	B	452	TYR	2.8
2	B	272	THR	2.7
2	D	309	ASN	2.7
2	B	400	SER	2.6
2	D	379	TYR	2.6
2	D	397	GLU	2.6
2	D	140	LEU	2.5
2	B	245	ASP	2.5
2	B	211	LEU	2.5
2	B	442	LEU	2.5
2	D	36	PHE	2.5
2	B	446	ALA	2.5
2	D	403	VAL	2.4
2	B	372	VAL	2.4
2	B	415	PHE	2.4
1	C	269	PHE	2.4
1	A	287	VAL	2.4
2	B	279	ARG	2.3
2	D	404	ILE	2.3
2	B	337	SER	2.3
2	B	309	ASN	2.3
2	B	437	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	384	LYS	2.3
1	A	229	LEU	2.3
2	D	452	TYR	2.3
1	A	445	LYS	2.3
2	B	312	ASP	2.3
2	B	356	ASN	2.3
2	D	454	VAL	2.2
2	B	333	GLU	2.2
2	D	359	ASP	2.2
1	A	289	ALA	2.2
2	B	282	GLN	2.2
2	D	388	ASP	2.2
1	C	266	TYR	2.1
2	D	145	PRO	2.1
2	D	408	TYR	2.1
2	D	375	ALA	2.1
2	D	382	GLU	2.1
2	B	9	VAL	2.0
2	B	364	SER	2.0
1	C	233	SER	2.0
2	D	383	LYS	2.0
2	B	194	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
3	CL	A	501	1/1	0.77	0.22	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	A	502	1/1	0.88	0.09	131,131,131,131	0
3	CL	C	501	1/1	0.92	0.54	164,164,164,164	0

6.5 Other polymers (i)

There are no such residues in this entry.