Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:10 PM UTC

PDB ID	:	1O6E / pdb_00001o6e
Title	:	Epstein-Barr virus protease
Authors	:	Buisson, M.; Hernandez, J.; Lascoux, D.; Schoehn, G.; Forest, E.; Arlaud, G.; Seigneurin, J.; Ruigrok, R.W.H.; Burmeister, W.P.
Deposited on	:	2002-09-13
Resolution	:	2.30 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:

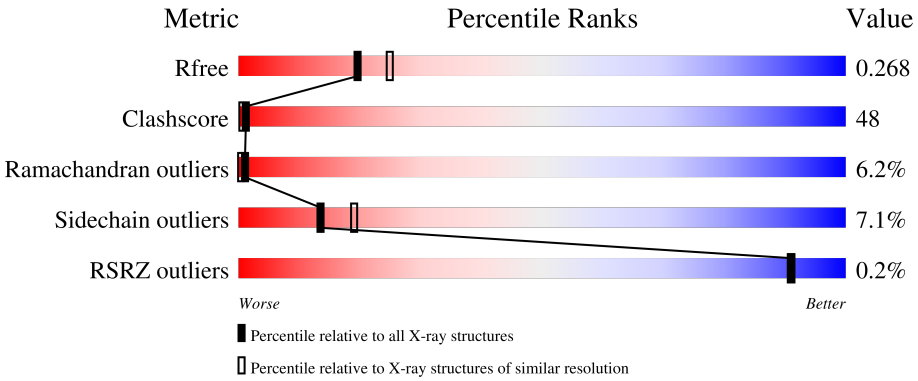
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	235	40% 46% 9% .
1	B	235	34% 53% 9% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3509 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.

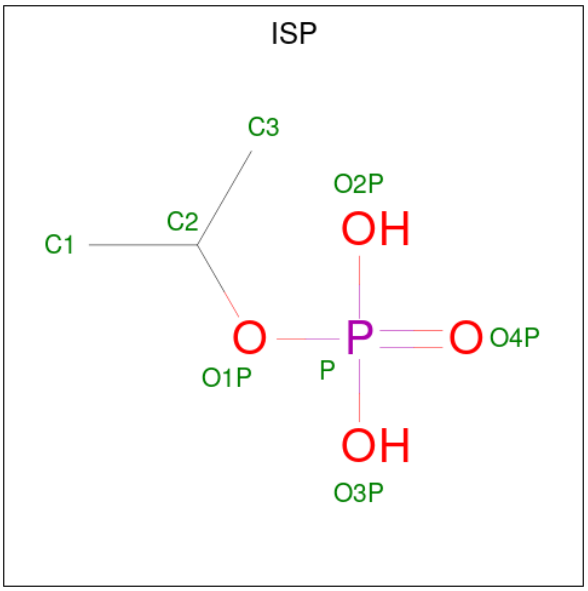
- Molecule 1 is a protein called CAPSID PROTEIN P40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1717	1096	298	319	4			
1	B	232	Total	C	N	O	S	0	0	0
			1766	1123	305	333	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	SER	ARG	engineered mutation	UNP P03234
B	64	SER	ARG	engineered mutation	UNP P03234

- Molecule 2 is PHOSPHORYLISOPROPANE (CCD ID: ISP) (formula: $C_3H_9O_4P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			7	3	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			7	3	3	1		

- Molecule 3 is water.

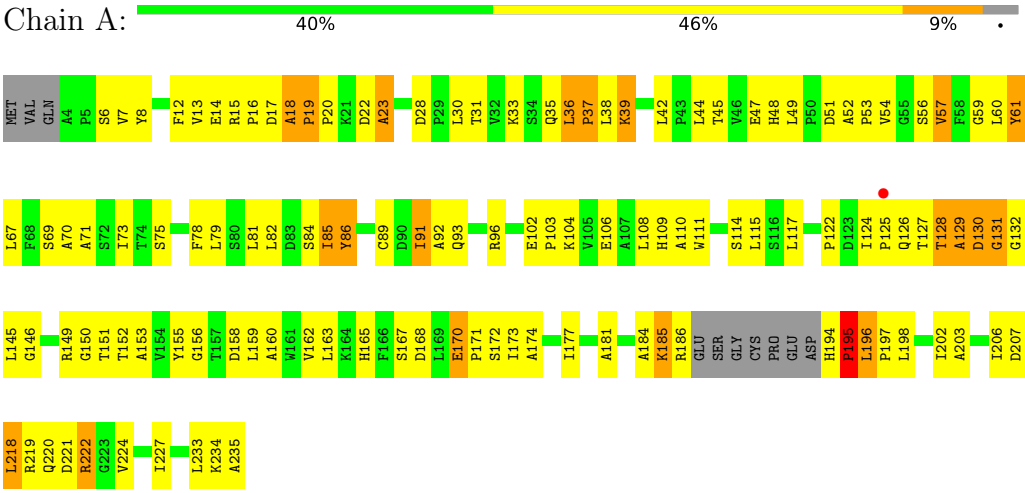
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	8	Total	O	0	0
			8	8		

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.

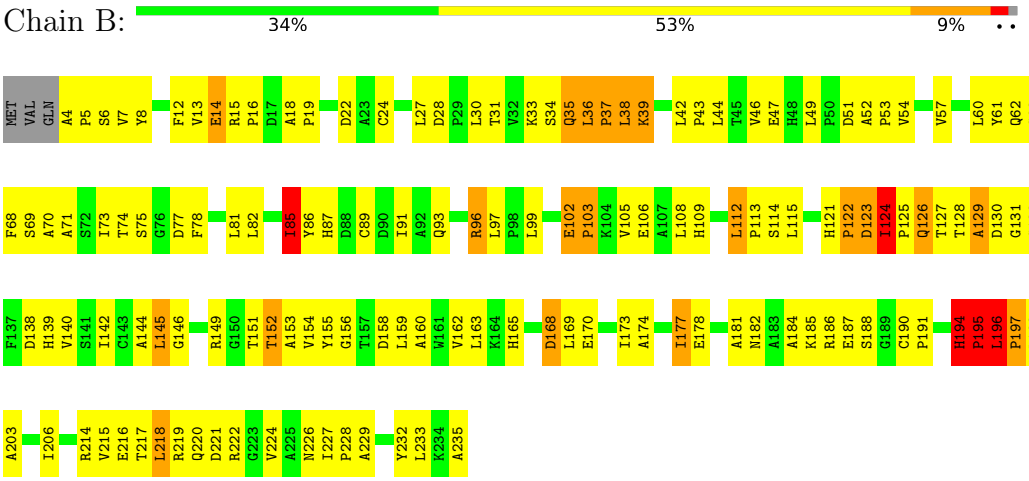
• Molecule 1: CAPSID PROTEIN P40

Chain A:



• Molecule 1: CAPSID PROTEIN P40

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	52.80Å 52.80Å 330.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.00 – 2.30 42.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (42.00-2.30) 98.1 (42.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.273 0.202 , 0.268	Depositor DCC
R_{free} test set	1232 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3509	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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 (i)

5.1 Standard geometry (i)

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

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	0.50	0/1760	1.17	12/2400 (0.5%)
1	B	0.54	0/1811	1.12	12/2471 (0.5%)
All	All	0.52	0/3571	1.14	24/4871 (0.5%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	LYS	N-CA-C	-12.40	84.40	110.80
1	B	124	ILE	CA-C-N	-8.66	111.20	120.47
1	B	124	ILE	C-N-CA	-8.66	111.20	120.47
1	B	112	LEU	CA-C-N	8.55	128.13	119.24
1	B	112	LEU	C-N-CA	8.55	128.13	119.24
1	A	19	PRO	N-CA-C	8.45	121.00	110.70
1	A	23	ALA	N-CA-C	8.32	121.92	111.69
1	A	19	PRO	CA-C-N	8.26	128.40	120.31
1	A	19	PRO	C-N-CA	8.26	128.40	120.31
1	A	18	ALA	CA-C-N	7.79	128.41	120.38
1	A	18	ALA	C-N-CA	7.79	128.41	120.38
1	B	64	SER	N-CA-C	-7.65	104.08	113.19
1	A	128	THR	N-CA-C	-7.33	95.23	108.58
1	A	86	TYR	N-CA-C	7.24	119.17	111.28
1	B	134	LEU	N-CA-C	6.89	119.96	110.24
1	B	86	TYR	N-CA-C	5.94	118.24	111.11
1	B	196	LEU	CA-C-N	5.80	127.09	119.84
1	B	196	LEU	C-N-CA	5.80	127.09	119.84
1	A	131	GLY	N-CA-C	-5.72	99.62	113.18
1	B	96	ARG	N-CA-C	-5.71	104.97	111.14
1	A	170	GLU	CA-C-N	5.57	125.92	119.47
1	A	170	GLU	C-N-CA	5.57	125.92	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	35	GLN	N-CA-C	-5.57	106.44	113.18
1	B	82	LEU	N-CA-C	-5.13	106.28	112.54

There are no chirality outliers.

There are no planarity outliers.

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	1717	0	1727	163	0
1	B	1766	0	1764	183	0
2	A	7	0	7	0	0
2	B	7	0	7	0	0
3	A	4	0	0	1	0
3	B	8	0	0	0	0
All	All	3509	0	3505	335	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 48.

All (335) 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:B:36:LEU:HB3	1:B:37:PRO:CD	1.75	1.15
1:B:36:LEU:HB3	1:B:37:PRO:HD2	1.27	1.15
1:A:36:LEU:HB3	1:A:37:PRO:HD2	1.15	1.13
1:A:30:LEU:HD13	1:A:132:GLY:HA2	1.33	1.10
1:A:36:LEU:HB3	1:A:37:PRO:CD	1.80	1.09
1:A:149:ARG:HH12	1:A:217:THR:CG2	1.69	1.06
1:A:149:ARG:HH12	1:A:217:THR:HG23	1.13	1.05
1:B:145:LEU:HD11	1:B:149:ARG:HH12	1.24	1.02
1:A:54:VAL:HG22	1:A:73:ILE:HG23	1.40	1.00
1:A:70:ALA:HB2	1:A:177:ILE:HD11	1.43	0.99
1:A:198:LEU:O	1:A:202:ILE:HD13	1.61	0.98
1:A:30:LEU:HB3	1:A:132:GLY:HA3	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:THR:HB	1:B:134:LEU:HB2	1.49	0.94
1:A:149:ARG:NH1	1:A:217:THR:HG23	1.87	0.88
1:B:33:LYS:O	1:B:36:LEU:HG	1.76	0.85
1:A:170:GLU:HB2	1:A:173:ILE:CD1	2.08	0.82
1:A:18:ALA:HB2	1:A:224:VAL:HG11	1.63	0.79
1:B:123:ASP:O	1:B:124:ILE:HB	1.82	0.79
1:A:70:ALA:CB	1:A:177:ILE:HD11	2.14	0.77
1:B:60:LEU:CD2	1:B:69:SER:HB3	2.14	0.77
1:B:31:THR:HG21	1:B:135:SER:HB3	1.67	0.77
1:A:195:PRO:O	1:A:196:LEU:HG	1.84	0.76
1:B:52:ALA:N	1:B:53:PRO:HD3	2.00	0.76
1:B:146:GLY:O	1:B:149:ARG:NH2	2.19	0.75
1:B:127:THR:HG22	1:B:128:THR:H	1.50	0.75
1:A:30:LEU:HD13	1:A:132:GLY:CA	2.13	0.75
1:B:174:ALA:O	1:B:178:GLU:HG3	1.87	0.74
1:A:202:ILE:HD12	1:B:202:ILE:HG12	1.69	0.74
1:A:89:CYS:O	1:A:93:GLN:HG3	1.88	0.74
1:B:128:THR:O	1:B:130:ASP:N	2.21	0.73
1:B:186:ARG:HG3	1:B:186:ARG:HH11	1.54	0.73
1:B:33:LYS:O	1:B:33:LYS:HG2	1.87	0.73
1:A:128:THR:O	1:A:130:ASP:N	2.21	0.73
1:A:115:LEU:H	1:A:151:THR:CG2	2.02	0.72
1:A:115:LEU:HG	1:A:153:ALA:HB2	1.72	0.72
1:B:197:PRO:HB2	1:B:200:LYS:HB2	1.70	0.72
1:B:16:PRO:O	1:B:19:PRO:HD3	1.90	0.72
1:A:128:THR:C	1:A:130:ASP:H	1.99	0.71
1:A:165:HIS:HB3	1:A:227:ILE:HG23	1.72	0.71
1:A:16:PRO:HD2	1:A:65:ALA:O	1.90	0.71
1:B:195:PRO:O	1:B:196:LEU:HG	1.88	0.71
1:B:60:LEU:HD23	1:B:69:SER:HB3	1.71	0.71
1:B:194:HIS:O	1:B:195:PRO:C	2.34	0.70
1:A:60:LEU:HD23	1:A:69:SER:HA	1.74	0.70
1:B:121:HIS:C	1:B:123:ASP:H	1.96	0.70
1:A:84:SER:HB3	1:B:199:THR:HG21	1.73	0.70
1:A:51:ASP:C	1:A:53:PRO:HD3	2.18	0.69
1:B:174:ALA:O	1:B:177:ILE:HG22	1.92	0.69
1:A:174:ALA:O	1:A:177:ILE:HG22	1.91	0.69
1:A:202:ILE:O	1:A:206:ILE:HG12	1.92	0.69
1:A:194:HIS:O	1:A:195:PRO:C	2.35	0.69
1:B:43:PRO:HD2	1:B:138:ASP:O	1.93	0.69
1:B:127:THR:HG22	1:B:128:THR:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:HD12	1:A:173:ILE:H	1.57	0.69
1:A:75:SER:O	1:A:79:LEU:HG	1.92	0.68
1:B:112:LEU:HD13	1:B:142:ILE:HD12	1.76	0.68
1:A:6:SER:HB2	1:A:73:ILE:O	1.94	0.68
1:A:152:THR:HB	1:A:221:ASP:HB3	1.76	0.67
1:B:16:PRO:HD2	1:B:65:ALA:O	1.95	0.66
1:B:145:LEU:HD22	1:B:218:LEU:HD13	1.77	0.66
1:A:30:LEU:CB	1:A:132:GLY:HA3	2.22	0.66
1:A:196:LEU:O	1:A:198:LEU:N	2.27	0.66
1:A:22:ASP:OD1	1:A:23:ALA:N	2.26	0.66
1:B:37:PRO:HB2	1:B:38:LEU:HD23	1.78	0.66
1:B:121:HIS:C	1:B:123:ASP:N	2.50	0.66
1:A:31:THR:O	1:A:35:GLN:HG2	1.95	0.66
1:A:115:LEU:H	1:A:151:THR:HG22	1.60	0.66
1:B:108:LEU:HD13	1:B:155:TYR:CD1	2.31	0.65
1:B:36:LEU:CB	1:B:37:PRO:HD2	2.16	0.65
1:B:96:ARG:CZ	1:B:222:ARG:NH1	2.60	0.65
1:B:216:GLU:HA	1:B:219:ARG:HD2	1.77	0.65
1:B:51:ASP:C	1:B:53:PRO:HD3	2.22	0.64
1:B:168:ASP:OD2	1:B:226:ASN:HB2	1.97	0.64
1:B:145:LEU:HD11	1:B:149:ARG:NH1	2.05	0.64
1:B:102:GLU:HB3	1:B:105:VAL:CG2	2.28	0.64
1:A:82:LEU:HD13	1:A:108:LEU:HG	1.81	0.63
1:B:7:VAL:HG12	1:B:8:TYR:N	2.12	0.63
1:B:102:GLU:O	1:B:106:GLU:HG3	1.97	0.63
1:B:122:PRO:O	1:B:125:PRO:HD2	1.98	0.63
1:A:60:LEU:HD21	1:A:69:SER:HB3	1.81	0.63
1:B:145:LEU:HD22	1:B:218:LEU:CD1	2.29	0.62
1:A:15:ARG:HB3	1:A:17:ASP:OD1	1.98	0.62
1:B:35:GLN:HE22	1:B:136:PHE:HA	1.64	0.62
1:B:202:ILE:O	1:B:206:ILE:HG12	1.99	0.62
1:A:152:THR:HG23	1:A:152:THR:O	2.00	0.61
1:A:109:HIS:CE1	1:A:155:TYR:HD2	2.18	0.61
1:B:22:ASP:CG	1:B:24:CYS:HG	2.07	0.61
1:B:36:LEU:CB	1:B:37:PRO:CD	2.65	0.61
1:A:52:ALA:N	1:A:53:PRO:HD3	2.16	0.60
1:B:75:SER:HB3	1:B:78:PHE:HB3	1.82	0.60
1:A:8:TYR:CD2	1:A:159:LEU:HG	2.35	0.60
1:B:38:LEU:HD23	1:B:38:LEU:H	1.66	0.60
1:A:42:LEU:HB3	1:A:57:VAL:HB	1.82	0.60
1:A:30:LEU:HB3	1:A:132:GLY:CA	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LEU:HB3	1:B:235:ALA:HB3	1.84	0.60
1:A:152:THR:HG21	1:A:222:ARG:HA	1.83	0.59
1:B:165:HIS:HB3	1:B:227:ILE:HG23	1.82	0.59
1:A:38:LEU:HD21	1:A:59:GLY:HA2	1.83	0.58
1:A:127:THR:O	1:A:129:ALA:N	2.35	0.58
1:A:38:LEU:CD2	1:A:59:GLY:HA2	2.34	0.58
1:B:220:GLN:O	1:B:224:VAL:HG23	2.03	0.57
1:A:61:TYR:O	1:A:67:LEU:HD12	2.04	0.57
1:A:51:ASP:HB2	1:A:194:HIS:CE1	2.40	0.57
1:B:121:HIS:O	1:B:123:ASP:N	2.37	0.57
1:B:165:HIS:O	1:B:227:ILE:HA	2.04	0.57
1:B:215:VAL:O	1:B:219:ARG:HG3	2.04	0.57
1:A:156:GLY:HA3	1:A:162:VAL:HG22	1.86	0.57
1:B:12:PHE:O	1:B:151:THR:HA	2.05	0.56
1:B:43:PRO:O	1:B:139:HIS:HB2	2.04	0.56
1:A:84:SER:CB	1:B:199:THR:HG21	2.34	0.56
1:A:108:LEU:HD13	1:A:155:TYR:CD1	2.40	0.56
1:B:122:PRO:O	1:B:123:ASP:O	2.24	0.56
1:A:195:PRO:O	1:A:196:LEU:CG	2.54	0.56
1:B:60:LEU:HD23	1:B:69:SER:CB	2.35	0.56
1:B:124:ILE:H	1:B:126:GLN:NE2	2.03	0.56
1:B:129:ALA:O	1:B:130:ASP:C	2.49	0.56
1:A:81:LEU:O	1:A:85:ILE:HG13	2.06	0.56
1:B:177:ILE:HD13	1:B:177:ILE:O	2.06	0.56
1:B:190:CYS:N	1:B:191:PRO:HD3	2.20	0.55
1:A:18:ALA:CB	1:A:224:VAL:HG11	2.34	0.55
1:B:195:PRO:O	1:B:196:LEU:CG	2.54	0.55
1:A:36:LEU:CB	1:A:37:PRO:HD2	2.10	0.55
1:A:181:ALA:O	1:A:185:LYS:HG3	2.07	0.55
1:B:63:SER:C	1:B:65:ALA:H	2.14	0.55
1:A:109:HIS:CD2	1:A:233:LEU:HD23	2.42	0.55
1:A:115:LEU:O	1:A:151:THR:HG21	2.07	0.55
1:B:87:HIS:HA	1:B:93:GLN:NE2	2.22	0.54
1:B:152:THR:HB	1:B:221:ASP:HB3	1.88	0.54
1:A:158:ASP:O	1:A:162:VAL:HG23	2.06	0.54
1:B:87:HIS:HA	1:B:93:GLN:HE21	1.72	0.54
1:A:13:VAL:HG21	1:A:117:LEU:HD22	1.88	0.54
1:A:30:LEU:CD1	1:A:132:GLY:HA2	2.20	0.54
1:B:70:ALA:CB	1:B:177:ILE:HD11	2.37	0.54
1:B:113:PRO:HD2	1:B:144:ALA:HA	1.88	0.54
1:B:127:THR:OG1	1:B:134:LEU:HD12	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:O	1:A:151:THR:CG2	2.55	0.54
1:B:109:HIS:CE1	1:B:233:LEU:HD23	2.43	0.54
1:A:198:LEU:O	1:A:202:ILE:CD1	2.47	0.54
1:A:61:TYR:OH	1:A:177:ILE:HG13	2.09	0.53
1:A:184:ALA:C	1:A:186:ARG:H	2.16	0.53
1:B:199:THR:O	1:B:202:ILE:HG22	2.09	0.53
1:A:18:ALA:HB2	1:A:224:VAL:CG1	2.37	0.53
1:B:15:ARG:NH1	1:B:224:VAL:O	2.41	0.53
1:A:129:ALA:C	1:A:131:GLY:N	2.66	0.53
1:A:202:ILE:CD1	1:B:202:ILE:HG12	2.37	0.53
1:A:15:ARG:HG2	1:A:15:ARG:HH11	1.73	0.53
1:A:86:TYR:CE1	1:A:93:GLN:HA	2.44	0.53
1:B:96:ARG:CZ	1:B:222:ARG:HH12	2.22	0.53
1:B:22:ASP:OD1	1:B:24:CYS:SG	2.60	0.52
1:B:105:VAL:HA	1:B:108:LEU:HD12	1.91	0.52
1:A:54:VAL:HG21	1:A:78:PHE:CD1	2.45	0.52
1:B:81:LEU:HD12	1:B:81:LEU:O	2.09	0.52
1:A:124:ILE:O	1:A:125:PRO:C	2.51	0.51
1:B:14:GLU:HG2	1:B:27:LEU:HD12	1.91	0.51
1:B:44:LEU:HD13	1:B:71:ALA:CB	2.40	0.51
1:A:33:LYS:O	1:A:36:LEU:HG	2.10	0.51
1:B:61:TYR:CZ	1:B:177:ILE:HG12	2.45	0.51
1:A:82:LEU:HB3	1:A:104:LYS:HA	1.92	0.51
1:A:124:ILE:CG1	1:A:125:PRO:HD2	2.40	0.51
1:B:162:VAL:O	1:B:165:HIS:HD2	1.93	0.51
1:B:174:ALA:HA	1:B:177:ILE:HG22	1.92	0.51
1:A:117:LEU:HD13	1:A:140:VAL:HG22	1.92	0.51
1:A:149:ARG:NE	1:A:149:ARG:HA	2.26	0.51
1:B:186:ARG:HG3	1:B:186:ARG:NH1	2.21	0.51
1:B:22:ASP:CG	1:B:24:CYS:SG	2.93	0.51
1:B:128:THR:HA	1:B:132:GLY:O	2.10	0.51
1:B:197:PRO:CB	1:B:200:LYS:HB2	2.41	0.51
1:A:198:LEU:HD12	1:B:198:LEU:HD12	1.93	0.51
1:B:154:VAL:HG12	1:B:162:VAL:HG13	1.94	0.50
1:B:52:ALA:N	1:B:53:PRO:CD	2.73	0.50
1:B:15:ARG:HH22	1:B:168:ASP:CG	2.18	0.50
1:A:60:LEU:CD2	1:A:69:SER:HB3	2.40	0.50
1:B:15:ARG:NH2	1:B:168:ASP:CG	2.70	0.50
1:B:125:PRO:O	1:B:126:GLN:O	2.29	0.50
1:B:42:LEU:HB2	1:B:57:VAL:HB	1.93	0.49
1:A:165:HIS:O	1:A:227:ILE:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HB2	1:B:52:ALA:HB3	1.94	0.49
1:B:184:ALA:C	1:B:186:ARG:H	2.19	0.49
1:A:38:LEU:HD21	1:A:59:GLY:CA	2.42	0.49
1:A:145:LEU:CD1	1:A:218:LEU:HD13	2.43	0.49
1:A:170:GLU:HB2	1:A:173:ILE:HD12	1.93	0.49
1:B:8:TYR:CD1	1:B:159:LEU:HD21	2.47	0.49
1:B:31:THR:O	1:B:35:GLN:HG2	2.12	0.49
1:B:102:GLU:HB3	1:B:105:VAL:HG22	1.94	0.49
1:B:18:ALA:HB2	1:B:224:VAL:HG11	1.94	0.49
1:B:38:LEU:H	1:B:38:LEU:CD2	2.26	0.49
1:A:8:TYR:CE2	1:A:159:LEU:HG	2.48	0.48
1:A:207:ASP:HA	1:B:91:ILE:HG13	1.94	0.48
1:B:63:SER:C	1:B:65:ALA:N	2.67	0.48
1:B:127:THR:CG2	1:B:128:THR:N	2.77	0.48
1:A:127:THR:C	1:A:129:ALA:N	2.71	0.48
1:B:123:ASP:O	1:B:124:ILE:CB	2.58	0.48
1:A:96:ARG:CZ	1:A:222:ARG:HH12	2.26	0.48
1:B:97:LEU:HD12	1:B:229:ALA:O	2.13	0.48
1:A:15:ARG:HH12	1:A:65:ALA:HB1	1.78	0.48
1:A:102:GLU:O	1:A:106:GLU:HG2	2.13	0.48
1:B:81:LEU:O	1:B:85:ILE:HB	2.14	0.48
1:B:124:ILE:H	1:B:126:GLN:HE21	1.61	0.48
1:B:145:LEU:HD23	1:B:214:ARG:HG3	1.96	0.48
1:A:36:LEU:CB	1:A:37:PRO:CD	2.71	0.47
1:B:31:THR:OG1	1:B:133:LYS:O	2.31	0.47
1:A:203:ALA:HB1	1:B:89:CYS:HB2	1.96	0.47
1:A:28:ASP:OD2	1:A:30:LEU:HD12	2.14	0.47
1:B:165:HIS:HB3	1:B:228:PRO:HD2	1.97	0.47
1:B:7:VAL:HG12	1:B:8:TYR:H	1.80	0.47
1:B:114:SER:CB	1:B:146:GLY:H	2.26	0.47
1:A:129:ALA:O	1:A:131:GLY:N	2.48	0.47
1:B:7:VAL:CG1	1:B:8:TYR:N	2.78	0.47
1:A:213:ASN:O	1:A:217:THR:OG1	2.30	0.47
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.80	0.47
1:B:15:ARG:NH2	1:B:65:ALA:HB1	2.29	0.47
1:B:60:LEU:HA	1:B:68:PHE:O	2.15	0.47
1:A:54:VAL:CG2	1:A:73:ILE:HG23	2.28	0.47
1:A:96:ARG:NH2	1:A:222:ARG:HH12	2.12	0.47
1:A:73:ILE:HG22	1:A:79:LEU:HD21	1.97	0.47
1:A:81:LEU:HG	1:A:85:ILE:CD1	2.45	0.46
1:B:145:LEU:HD12	1:B:146:GLY:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:HG22	1:A:73:ILE:CG2	2.29	0.46
1:A:216:GLU:O	1:A:220:GLN:HG3	2.14	0.46
1:B:220:GLN:HE21	1:B:224:VAL:HG21	1.81	0.46
1:B:78:PHE:HB2	1:B:196:LEU:HD11	1.97	0.46
1:B:159:LEU:O	1:B:160:ALA:C	2.59	0.46
1:A:149:ARG:C	1:A:151:THR:H	2.23	0.46
1:B:6:SER:HB2	1:B:73:ILE:O	2.16	0.46
1:A:114:SER:CB	1:A:146:GLY:H	2.29	0.46
1:B:30:LEU:HD23	1:B:30:LEU:HA	1.71	0.46
1:A:28:ASP:C	1:A:30:LEU:H	2.24	0.46
1:B:4:ALA:N	1:B:5:PRO:HD3	2.30	0.46
1:A:28:ASP:HB3	1:A:30:LEU:HD12	1.98	0.45
1:A:44:LEU:HD22	1:A:71:ALA:HB1	1.97	0.45
1:B:174:ALA:C	1:B:177:ILE:HG22	2.40	0.45
1:A:222:ARG:HG2	1:A:222:ARG:NH1	2.31	0.45
1:B:38:LEU:HD23	1:B:38:LEU:N	2.30	0.45
1:A:216:GLU:OE1	1:A:216:GLU:N	2.42	0.45
1:A:218:LEU:HB3	1:A:235:ALA:HB3	1.97	0.45
1:A:12:PHE:O	1:A:151:THR:HA	2.17	0.45
1:A:42:LEU:HB3	1:A:57:VAL:CG2	2.46	0.45
1:B:174:ALA:HA	1:B:177:ILE:CG2	2.45	0.45
1:A:47:GLU:O	1:A:48:HIS:HB2	2.17	0.45
1:A:61:TYR:CZ	1:A:177:ILE:HG13	2.51	0.45
1:B:62:GLN:O	1:B:173:ILE:HD11	2.16	0.45
1:B:159:LEU:HD11	1:B:181:ALA:HB2	1.98	0.45
1:B:112:LEU:HD13	1:B:142:ILE:CD1	2.44	0.45
1:B:36:LEU:HB3	1:B:37:PRO:HD3	1.86	0.45
1:A:63:SER:C	1:A:65:ALA:N	2.74	0.44
1:A:15:ARG:HD3	1:A:150:GLY:HA3	1.99	0.44
1:A:28:ASP:C	1:A:30:LEU:N	2.73	0.44
1:A:159:LEU:HA	1:A:162:VAL:HB	1.99	0.44
1:A:42:LEU:HB3	1:A:57:VAL:CB	2.48	0.44
1:A:111:TRP:CD1	1:B:206:ILE:CD1	3.00	0.44
1:B:127:THR:CG2	1:B:128:THR:H	2.22	0.44
1:A:60:LEU:HD23	1:A:69:SER:CA	2.44	0.44
1:B:38:LEU:O	1:B:39:LYS:C	2.57	0.44
1:A:173:ILE:HD12	1:A:173:ILE:N	2.27	0.44
1:A:233:LEU:HB3	3:A:2004:HOH:O	2.18	0.44
1:B:156:GLY:HA3	1:B:162:VAL:CG2	2.48	0.44
1:A:45:THR:O	1:A:141:SER:HA	2.18	0.44
1:B:112:LEU:HD22	1:B:142:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:C	1:A:19:PRO:HD3	2.43	0.43
1:B:99:LEU:HD13	1:B:232:TYR:CE2	2.54	0.43
1:A:18:ALA:N	1:A:19:PRO:HD3	2.32	0.43
1:B:202:ILE:CD1	1:B:206:ILE:HD11	2.48	0.43
1:A:222:ARG:HG2	1:A:222:ARG:HH11	1.83	0.43
1:B:156:GLY:HA3	1:B:162:VAL:HG22	2.00	0.43
1:B:13:VAL:CG2	1:B:67:LEU:HD23	2.48	0.43
1:B:37:PRO:HB2	1:B:38:LEU:H	1.53	0.43
1:B:122:PRO:O	1:B:123:ASP:C	2.60	0.43
1:B:196:LEU:O	1:B:198:LEU:N	2.51	0.43
1:A:89:CYS:HB3	1:A:92:ALA:HB3	2.00	0.43
1:A:159:LEU:O	1:A:160:ALA:C	2.61	0.43
1:B:227:ILE:HG23	1:B:228:PRO:HD2	2.01	0.43
1:B:127:THR:CB	1:B:134:LEU:HD12	2.48	0.43
1:A:15:ARG:HG2	1:A:15:ARG:NH1	2.34	0.43
1:A:124:ILE:HG13	1:A:125:PRO:HD2	1.99	0.43
1:A:110:ALA:HB2	1:A:234:LYS:HG3	2.00	0.43
1:B:4:ALA:N	1:B:5:PRO:CD	2.82	0.43
1:B:194:HIS:O	1:B:196:LEU:N	2.51	0.43
1:A:174:ALA:HA	1:A:177:ILE:HG22	2.00	0.42
1:B:57:VAL:HG21	1:B:140:VAL:HB	1.99	0.42
1:A:149:ARG:HA	1:A:149:ARG:HE	1.84	0.42
1:A:219:ARG:NH1	1:A:219:ARG:CB	2.82	0.42
1:B:44:LEU:HD13	1:B:71:ALA:HB1	2.00	0.42
1:B:122:PRO:HG2	1:B:134:LEU:HD13	2.01	0.42
1:A:159:LEU:HB3	1:A:163:LEU:HD12	2.02	0.42
1:B:28:ASP:C	1:B:30:LEU:N	2.77	0.42
1:B:61:TYR:OH	1:B:177:ILE:HG12	2.19	0.42
1:A:184:ALA:O	1:A:186:ARG:N	2.52	0.42
1:A:222:ARG:CB	1:A:233:LEU:CD1	2.97	0.42
1:B:122:PRO:O	1:B:125:PRO:CD	2.66	0.42
1:B:149:ARG:NH1	1:B:217:THR:HG22	2.34	0.42
1:B:182:ASN:N	1:B:182:ASN:HD22	2.17	0.42
1:A:35:GLN:O	1:A:39:LYS:HE3	2.19	0.42
1:A:122:PRO:CB	1:A:126:GLN:HB2	2.49	0.42
1:A:124:ILE:HG12	1:A:125:PRO:HD2	2.01	0.42
1:B:128:THR:HG22	1:B:131:GLY:H	1.85	0.42
1:A:54:VAL:HG22	1:A:54:VAL:O	2.20	0.42
1:B:47:GLU:OE2	1:B:47:GLU:HA	2.19	0.42
1:B:158:ASP:OD1	1:B:158:ASP:N	2.53	0.42
1:B:202:ILE:HD12	1:B:206:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LEU:HA	1:B:197:PRO:HD3	1.86	0.42
1:B:13:VAL:HG13	1:B:69:SER:OG	2.21	0.41
1:A:117:LEU:HD13	1:A:140:VAL:CG2	2.51	0.41
1:B:44:LEU:HD23	1:B:54:VAL:HG23	2.03	0.41
1:B:163:LEU:HD22	1:B:169:LEU:CD2	2.51	0.41
1:B:38:LEU:O	1:B:38:LEU:HG	2.20	0.41
1:B:202:ILE:CG2	1:B:203:ALA:N	2.82	0.41
1:A:129:ALA:O	1:A:130:ASP:C	2.62	0.41
1:A:202:ILE:CG2	1:B:85:ILE:HD11	2.51	0.41
1:A:219:ARG:HH11	1:A:219:ARG:CB	2.33	0.41
1:A:170:GLU:HA	1:A:171:PRO:HD3	1.85	0.41
1:A:219:ARG:O	1:A:222:ARG:HG3	2.20	0.41
1:B:31:THR:O	1:B:34:SER:HB3	2.20	0.41
1:B:18:ALA:HB1	1:B:149:ARG:HB2	2.02	0.41
1:B:60:LEU:HD23	1:B:69:SER:HA	2.03	0.41
1:B:109:HIS:O	1:B:113:PRO:HG3	2.20	0.41
1:B:177:ILE:HD13	1:B:177:ILE:C	2.46	0.41
1:A:7:VAL:HG13	1:A:156:GLY:O	2.21	0.41
1:A:48:HIS:HA	1:A:141:SER:OG	2.20	0.41
1:A:91:ILE:HG22	1:A:110:ALA:HB1	2.03	0.41
1:B:18:ALA:N	1:B:19:PRO:CD	2.84	0.41
1:B:51:ASP:OD2	1:B:200:LYS:HD2	2.21	0.41
1:B:99:LEU:HB3	1:B:232:TYR:CZ	2.55	0.41
1:B:70:ALA:HB1	1:B:177:ILE:HD11	2.03	0.41
1:A:202:ILE:HG21	1:B:85:ILE:HD11	2.01	0.40
1:B:115:LEU:HG	1:B:153:ALA:HB2	2.03	0.40
1:A:184:ALA:C	1:A:186:ARG:N	2.79	0.40
1:B:46:VAL:HB	1:B:52:ALA:HB1	2.04	0.40
1:B:186:ARG:O	1:B:187:GLU:C	2.65	0.40
1:A:109:HIS:CE1	1:A:155:TYR:CD2	3.06	0.40
1:A:170:GLU:HB2	1:A:173:ILE:HD11	1.97	0.40
1:B:63:SER:HA	1:B:170:GLU:OE1	2.21	0.40
1:A:49:LEU:HB2	1:A:52:ALA:HB3	2.03	0.40
1:A:111:TRP:CD1	1:B:206:ILE:HD11	2.56	0.40
1:A:152:THR:HG21	1:A:221:ASP:C	2.46	0.40
1:A:19:PRO:HA	1:A:20:PRO:HD3	1.74	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	221/235 (94%)	189 (86%)	20 (9%)	12 (5%)	1	1
1	B	230/235 (98%)	199 (86%)	15 (6%)	16 (7%)	1	0
All	All	451/470 (96%)	388 (86%)	35 (8%)	28 (6%)	1	0

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	PRO
1	A	103	PRO
1	A	129	ALA
1	A	196	LEU
1	A	197	PRO
1	B	36	LEU
1	B	103	PRO
1	B	123	ASP
1	B	124	ILE
1	B	126	GLN
1	B	129	ALA
1	B	188	SER
1	B	195	PRO
1	B	196	LEU
1	A	36	LEU
1	A	168	ASP
1	A	185	LYS
1	A	195	PRO
1	B	185	LYS
1	A	130	ASP
1	B	37	PRO
1	B	38	LEU
1	B	194	HIS
1	A	167	SER
1	B	197	PRO

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Mol	Chain	Res	Type
1	B	85	ILE
1	A	85	ILE
1	B	122	PRO

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	187/196 (95%)	176 (94%)	11 (6%)	18	26
1	B	193/196 (98%)	177 (92%)	16 (8%)	10	14
All	All	380/392 (97%)	353 (93%)	27 (7%)	13	19

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	56	SER
1	A	57	VAL
1	A	61	TYR
1	A	91	ILE
1	A	142	ILE
1	A	172	SER
1	A	195	PRO
1	A	216	GLU
1	A	218	LEU
1	A	222	ARG
1	B	14	GLU
1	B	39	LYS
1	B	74	THR
1	B	77	ASP
1	B	85	ILE
1	B	102	GLU
1	B	103	PRO
1	B	124	ILE
1	B	145	LEU

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Mol	Chain	Res	Type
1	B	152	THR
1	B	168	ASP
1	B	177	ILE
1	B	194	HIS
1	B	195	PRO
1	B	202	ILE
1	B	218	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	165	HIS
1	A	179	ASN
1	B	35	GLN
1	B	93	GLN
1	B	109	HIS
1	B	121	HIS
1	B	126	GLN
1	B	165	HIS
1	B	182	ASN
1	B	220	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	ISP	A	1236	1	4,6,7	1.16	1 (25%)	3,7,10	0.91	0
2	ISP	B	1236	1	4,6,7	1.20	1 (25%)	3,7,10	0.97	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	ISP	A	1236	1	-	0/2/4/5	-
2	ISP	B	1236	1	-	0/2/4/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1236	ISP	P-O1P	-2.20	1.56	1.62
2	A	1236	ISP	P-O1P	-2.10	1.57	1.62

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	225/235 (95%)	-0.68	1 (0%) 88 89	35, 61, 119, 145	0
1	B	232/235 (98%)	-0.85	0 100 100	28, 54, 104, 137	0
All	All	457/470 (97%)	-0.77	1 (0%) 91 91	28, 58, 113, 145	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	PRO	2.9

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 oligosaccharides in this entry.

6.4 Ligands

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
2	ISP	B	1236	7/8	0.99	0.06	51,51,53,54	0
2	ISP	A	1236	7/8	1.00	0.03	41,45,48,50	0

6.5 Other polymers (i)

There are no such residues in this entry.