Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:25 am BST

PDB ID	:	2P3V
Title	:	Thermotoga maritima IMPase TM1415
Authors	:	Stieglitz, K.A.; Roberts, M.F.; Li, W.; Stec, B.
Deposited on	:	2007-03-09
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

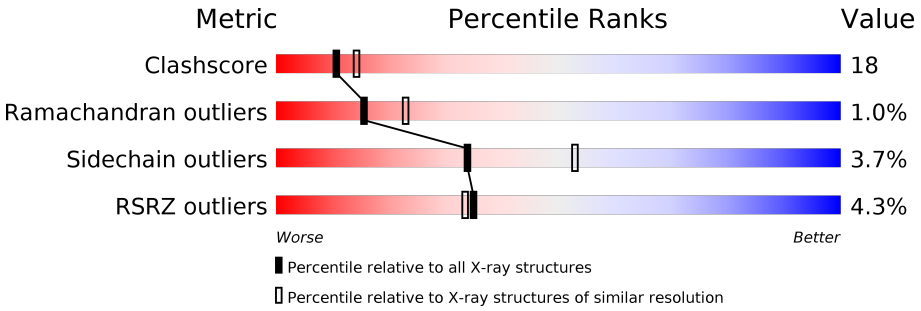
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	256	4% 65% 32%
1	B	256	4% 67% 29%
1	C	256	67% 30%
1	D	256	9% 58% 39%

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	SRT	B	4501	X	-	-	-
2	SRT	B	4502	X	-	-	-
2	SRT	C	4504	X	-	-	-
2	SRT	D	4503	X	-	-	-

2 Entry composition

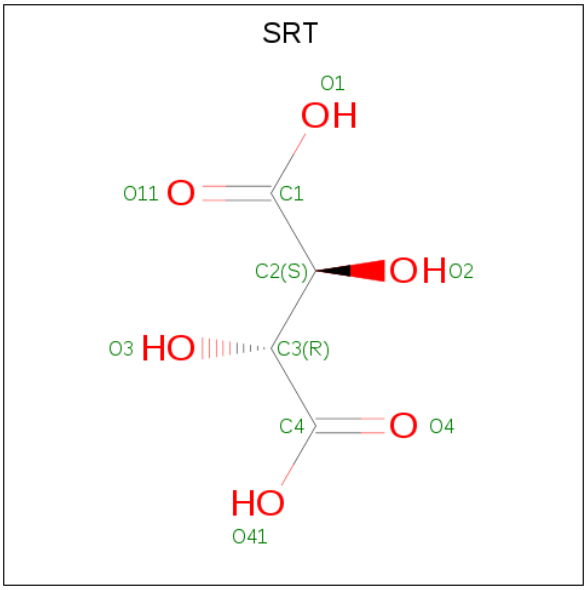
There are 3 unique types of molecules in this entry. The entry contains 8365 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Inositol-1-monophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2007	1281	345	374	7			
1	B	254	Total	C	N	O	S	0	0	0
			2007	1281	345	374	7			
1	C	254	Total	C	N	O	S	0	0	0
			2007	1281	345	374	7			
1	D	254	Total	C	N	O	S	0	0	0
			2007	1281	345	374	7			

- Molecule 2 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O		0	0
			10	4	6			
2	B	1	Total	C	O		0	0
			10	4	6			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0

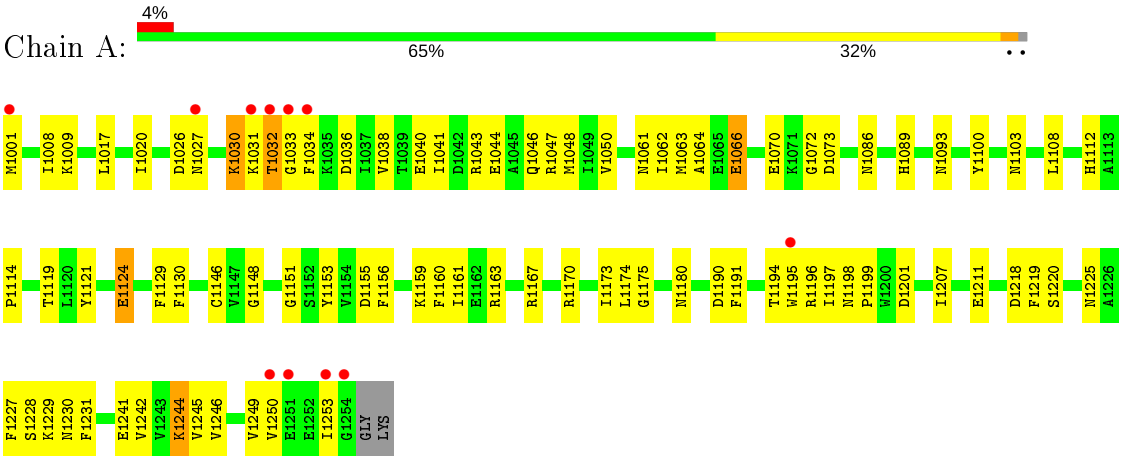
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	76	Total O 76 76	0	0
3	B	87	Total O 87 87	0	0
3	C	75	Total O 75 75	0	0
3	D	59	Total O 59 59	0	0

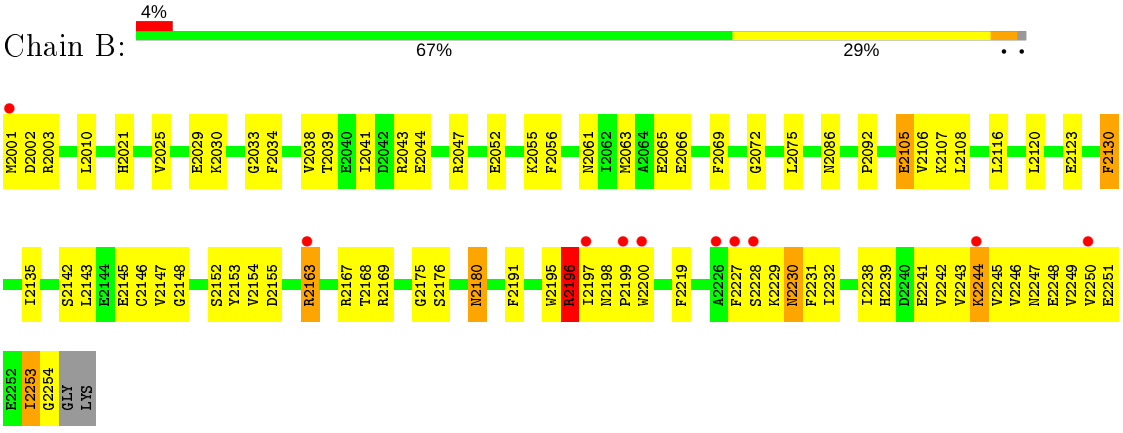
3 Residue-property plots (i)

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

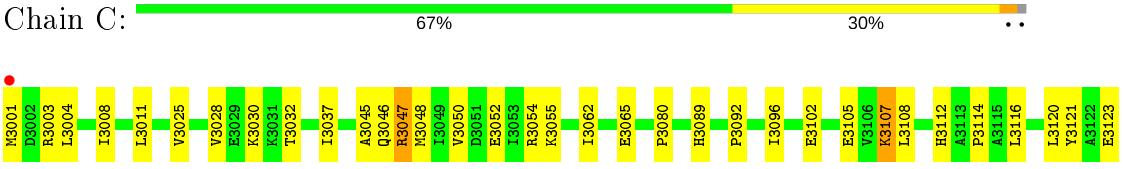
• Molecule 1: Inositol-1-monophosphatase

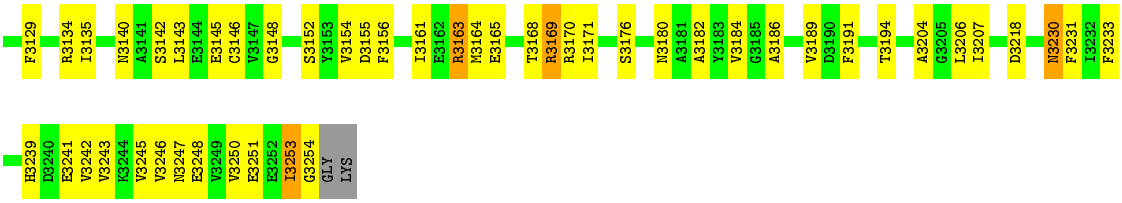


• Molecule 1: Inositol-1-monophosphatase



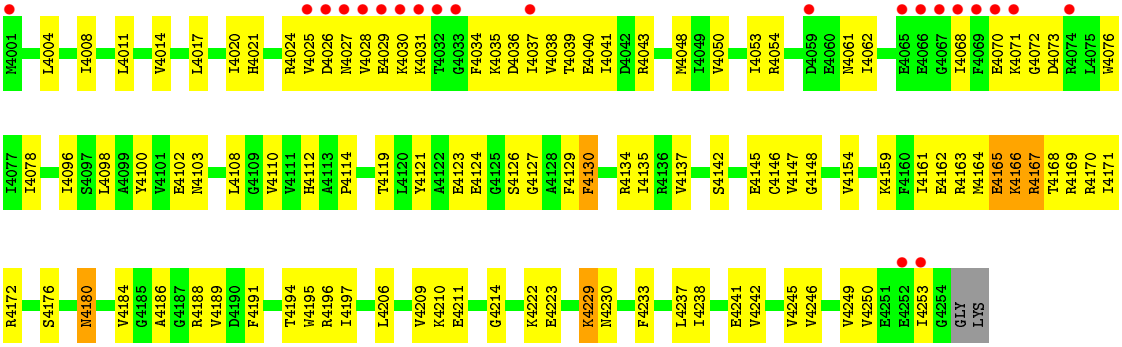
• Molecule 1: Inositol-1-monophosphatase





• Molecule 1: Inositol-1-monophosphatase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.81Å 97.94Å 122.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.40 34.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.0 (45.00-2.40) 88.3 (34.76-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.263 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 85.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8365	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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: SRT

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	0.40	0/2045	0.62	0/2757
1	B	0.39	0/2045	0.62	0/2757
1	C	0.40	0/2045	0.63	0/2757
1	D	0.38	0/2045	0.61	0/2757
All	All	0.39	0/8180	0.62	0/11028

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	2007	0	1990	69	0
1	B	2007	0	1990	77	0
1	C	2007	0	1990	61	0
1	D	2007	0	1990	99	0
2	B	20	0	8	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
3	A	76	0	0	2	0
3	B	87	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	75	0	0	1	0
3	D	59	0	0	2	0
All	All	8365	0	7976	295	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 18.

All (295) 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:2196:ARG:HH21	1:B:2229:LYS:HZ3	1.16	0.91
1:B:2196:ARG:HH21	1:B:2229:LYS:NZ	1.76	0.84
1:D:4027:ASN:HA	1:D:4030:LYS:HB3	1.59	0.84
1:D:4229:LYS:HD2	1:D:4230:ASN:H	1.43	0.84
1:D:4167:ARG:HH11	1:D:4167:ARG:HB3	1.46	0.81
1:D:4167:ARG:HB3	1:D:4167:ARG:NH1	1.94	0.80
1:B:2010:LEU:HD13	1:B:2052:GLU:HG2	1.63	0.80
1:A:1198:ASN:O	1:A:1201:ASP:HB2	1.84	0.78
1:C:3164:MET:O	1:C:3168:THR:HG22	1.84	0.76
1:C:3247:ASN:O	1:C:3251:GLU:HG2	1.86	0.76
1:C:3218:ASP:HB2	1:C:3230:ASN:OD1	1.90	0.72
1:B:2196:ARG:HG3	1:B:2229:LYS:HZ3	1.54	0.72
1:A:1093:ASN:HD22	1:A:1174:LEU:HB3	1.54	0.71
1:B:2105:GLU:OE2	1:B:2107:LYS:HE2	1.91	0.71
1:D:4229:LYS:HD2	1:D:4230:ASN:N	2.06	0.70
1:B:2230:ASN:HD22	1:B:2230:ASN:H	1.39	0.70
1:D:4129:PHE:CE2	1:D:4134:ARG:HD2	2.28	0.69
1:A:1031:LYS:HG3	1:A:1032:THR:H	1.58	0.68
1:A:1197:ILE:O	1:A:1197:ILE:HD12	1.94	0.68
1:D:4161:ILE:O	1:D:4165:GLU:HB3	1.94	0.68
1:A:1001:MET:HB2	3:A:5050:HOH:O	1.94	0.67
1:D:4011:LEU:HD12	1:D:4110:VAL:HG12	1.77	0.66
1:B:2163:ARG:HH12	1:B:2167:ARG:HD3	1.60	0.66
1:B:2247:ASN:HA	1:B:2250:VAL:HG12	1.78	0.65
1:D:4184:VAL:HG22	1:D:4189:VAL:HG23	1.78	0.65
1:A:1161:ILE:HD11	1:A:1173:ILE:HD11	1.79	0.64
1:D:4170:ARG:HG2	1:D:4172:ARG:NH2	2.12	0.64
1:D:4004:LEU:HD22	1:D:4123:GLU:HG3	1.79	0.64
1:B:2229:LYS:O	1:B:2229:LYS:HD3	1.99	0.63
1:A:1009:LYS:HD3	1:D:4024:ARG:HH12	1.64	0.63
1:B:2163:ARG:HD2	1:B:2245:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3054:ARG:HG3	1:C:3054:ARG:HH21	1.63	0.63
1:D:4025:VAL:HG13	1:D:4037:ILE:HG21	1.81	0.63
1:D:4031:LYS:HB3	1:D:4031:LYS:NZ	2.16	0.61
1:D:4229:LYS:HD3	1:D:4230:ASN:ND2	2.16	0.61
1:C:3102:GLU:HB2	1:C:3107:LYS:HD3	1.83	0.61
1:D:4030:LYS:HA	1:D:4034:PHE:HB3	1.83	0.61
1:A:1121:TYR:CE2	1:A:1129:PHE:HB2	2.36	0.60
1:D:4068:ILE:HG13	1:D:4070:GLU:HG3	1.83	0.60
1:B:2248:GLU:O	1:B:2251:GLU:HG2	2.01	0.60
1:C:3092:PRO:HD3	1:D:4188:ARG:NH1	2.16	0.60
1:C:3246:VAL:O	1:C:3250:VAL:HG23	2.01	0.59
1:D:4246:VAL:O	1:D:4250:VAL:HG23	2.02	0.59
1:D:4121:TYR:CE1	1:D:4129:PHE:HB2	2.38	0.59
1:A:1146:CYS:HA	1:A:1190:ASP:OD2	2.02	0.58
1:C:3163:ARG:HH12	1:C:3248:GLU:CB	2.16	0.58
1:D:4021:HIS:CD2	1:D:4041:ILE:HD12	2.38	0.58
1:A:1148:GLY:HA3	1:A:1191:PHE:CZ	2.38	0.58
1:C:3148:GLY:HA3	1:C:3191:PHE:CE1	2.38	0.58
1:A:1225:ASN:HD21	1:A:1227:PHE:HB2	1.68	0.58
1:B:2086:ASN:HD21	1:B:2175:GLY:HA3	1.68	0.58
1:D:4034:PHE:O	1:D:4038:VAL:HG23	2.03	0.58
1:C:3165:GLU:HG2	1:D:4154:VAL:HG13	1.84	0.58
1:B:2148:GLY:HA3	1:B:2191:PHE:CZ	2.39	0.58
1:D:4164:MET:O	1:D:4168:THR:HG22	2.04	0.58
1:B:2142:SER:O	1:B:2145:GLU:HG2	2.04	0.58
1:B:2001:MET:SD	1:B:2002:ASP:N	2.77	0.57
1:A:1031:LYS:HG3	1:A:1032:THR:N	2.19	0.57
1:C:3152:SER:HB3	1:D:4170:ARG:HD2	1.86	0.57
1:D:4034:PHE:O	1:D:4037:ILE:HG22	2.05	0.57
1:D:4206:LEU:O	1:D:4210:LYS:HG3	2.04	0.57
1:B:2196:ARG:HG3	1:B:2229:LYS:NZ	2.19	0.57
1:D:4229:LYS:HD3	1:D:4230:ASN:HD22	1.68	0.56
1:B:2063:MET:HE3	1:B:2075:LEU:HD21	1.86	0.56
1:A:1225:ASN:ND2	1:A:1227:PHE:HB2	2.20	0.56
1:C:3242:VAL:O	1:C:3246:VAL:HG23	2.06	0.56
1:D:4194:THR:HG21	1:D:4197:ILE:HD13	1.88	0.55
1:D:4137:VAL:HG11	1:D:4214:GLY:CA	2.36	0.55
1:D:4229:LYS:H	1:D:4229:LYS:HD2	1.70	0.55
1:B:2196:ARG:HG3	1:B:2229:LYS:HE2	1.89	0.55
1:B:2230:ASN:N	1:B:2230:ASN:HD22	2.01	0.55
1:C:3142:SER:O	1:C:3145:GLU:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4163:ARG:HD3	1:D:4249:VAL:HG22	1.88	0.55
1:D:4135:ILE:HB	1:D:4186:ALA:HA	1.88	0.55
1:B:2030:LYS:HB3	1:B:2033:GLY:O	2.07	0.55
1:B:2143:LEU:HD23	1:B:2167:ARG:HG2	1.89	0.55
1:B:2249:VAL:O	1:B:2253:ILE:HG13	2.07	0.54
1:C:3152:SER:HB3	1:D:4170:ARG:CD	2.36	0.54
1:B:2143:LEU:HD23	1:B:2167:ARG:CG	2.38	0.54
1:B:2167:ARG:HH12	1:B:2244:LYS:NZ	2.05	0.54
1:D:4031:LYS:HB3	1:D:4031:LYS:HZ3	1.71	0.54
1:A:1047:ARG:HD3	3:A:5307:HOH:O	2.07	0.54
1:C:3052:GLU:OE1	1:C:3055:LYS:HD2	2.08	0.54
1:D:4011:LEU:HD12	1:D:4110:VAL:CG1	2.38	0.54
1:D:4108:LEU:C	1:D:4108:LEU:HD12	2.27	0.54
1:A:1246:VAL:O	1:A:1250:VAL:HG23	2.07	0.54
1:A:1017:LEU:HD22	1:A:1048:MET:CE	2.38	0.53
1:A:1195:TRP:O	1:A:1197:ILE:HG23	2.08	0.53
1:D:4112:HIS:O	1:D:4114:PRO:HD3	2.09	0.53
1:A:1046:GLN:NE2	1:A:1064:ALA:HB1	2.24	0.53
1:B:2232:ILE:HD12	1:B:2243:VAL:HG22	1.90	0.53
1:C:3001:MET:N	1:C:3123:GLU:OE1	2.42	0.53
1:B:2199:PRO:HG3	1:B:2227:PHE:HB3	1.90	0.53
1:C:3129:PHE:CE2	1:C:3134:ARG:HD3	2.43	0.53
1:A:1073:ASP:HB2	1:A:1103:ASN:HD22	1.73	0.53
1:A:1163:ARG:HD2	1:A:1249:VAL:HG22	1.91	0.53
1:B:2167:ARG:HH12	1:B:2244:LYS:HZ1	1.55	0.53
1:B:2065:GLU:HG3	3:B:5289:HOH:O	2.08	0.53
1:D:4061:ASN:ND2	1:D:4072:GLY:HA3	2.25	0.52
1:A:1009:LYS:HE2	3:C:5342:HOH:O	2.08	0.52
1:C:3163:ARG:HH12	1:C:3248:GLU:HB3	1.75	0.52
1:C:3003:ARG:HB3	1:C:3108:LEU:HD21	1.92	0.52
1:D:4241:GLU:O	1:D:4245:VAL:HG23	2.09	0.52
1:A:1249:VAL:O	1:A:1253:ILE:HG23	2.10	0.52
1:B:2163:ARG:CD	1:B:2245:VAL:HG13	2.40	0.52
1:B:2245:VAL:O	1:B:2249:VAL:HG23	2.09	0.52
1:D:4196:ARG:N	1:D:4230:ASN:OD1	2.43	0.52
1:B:2230:ASN:ND2	1:B:2230:ASN:H	2.07	0.51
1:C:3107:LYS:N	1:C:3107:LYS:HD2	2.24	0.51
1:A:1044:GLU:HG2	1:A:1047:ARG:NH2	2.25	0.51
1:B:2196:ARG:NH2	1:B:2229:LYS:NZ	2.53	0.51
1:D:4166:LYS:HD3	1:D:4167:ARG:HG2	1.93	0.51
1:A:1017:LEU:HD22	1:A:1048:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2055:LYS:HD3	1:B:2056:PHE:CE1	2.45	0.51
1:B:2219:PHE:HB2	1:B:2230:ASN:OD1	2.10	0.51
1:D:4102:GLU:O	1:D:4103:ASN:HB2	2.10	0.51
1:B:2065:GLU:HA	1:B:2200:TRP:CD2	2.46	0.50
1:D:4054:ARG:HG2	1:D:4054:ARG:HH21	1.76	0.50
1:B:2242:VAL:O	1:B:2246:VAL:HG23	2.12	0.50
1:C:3169:ARG:O	1:C:3170:ARG:HD2	2.11	0.50
1:B:2196:ARG:HG3	1:B:2229:LYS:CE	2.42	0.50
1:B:2230:ASN:ND2	1:B:2230:ASN:N	2.59	0.50
1:C:3161:ILE:O	1:C:3165:GLU:HB2	2.11	0.50
1:A:1242:VAL:O	1:A:1246:VAL:HG23	2.11	0.50
1:D:4164:MET:HB3	1:D:4171:ILE:HD11	1.93	0.50
1:A:1030:LYS:O	1:A:1030:LYS:HE3	2.12	0.50
1:A:1093:ASN:ND2	1:A:1174:LEU:HB3	2.25	0.50
1:C:3143:LEU:HD11	1:C:3241:GLU:HB3	1.94	0.50
1:D:4176:SER:HB3	3:D:5319:HOH:O	2.12	0.50
1:A:1170:ARG:HD2	1:B:2152:SER:HB2	1.94	0.49
1:A:1124:GLU:HA	1:A:1211:GLU:OE1	2.12	0.49
1:B:2086:ASN:ND2	1:B:2175:GLY:HA3	2.27	0.49
1:B:2065:GLU:HA	1:B:2200:TRP:CE2	2.47	0.49
1:A:1250:VAL:HA	1:A:1253:ILE:HG12	1.94	0.49
1:B:2163:ARG:HD2	1:B:2245:VAL:CG1	2.42	0.49
1:D:4034:PHE:HA	1:D:4037:ILE:HG22	1.92	0.49
1:D:4127:GLY:HA3	1:D:4134:ARG:NH2	2.27	0.49
1:B:2154:VAL:O	1:B:2155:ASP:HB2	2.13	0.49
1:B:2247:ASN:HA	1:B:2250:VAL:CG1	2.42	0.49
1:C:3168:THR:HG21	1:C:3171:ILE:HD11	1.94	0.49
1:D:4170:ARG:HG2	1:D:4172:ARG:HH22	1.73	0.49
1:D:4100:TYR:HB3	1:D:4108:LEU:HG	1.94	0.49
1:C:3025:VAL:O	1:C:3030:LYS:HE3	2.13	0.49
1:C:3054:ARG:HG3	1:C:3054:ARG:NH2	2.26	0.49
1:C:3135:ILE:HB	1:C:3186:ALA:HA	1.94	0.49
1:D:4025:VAL:CG1	1:D:4034:PHE:HB2	2.43	0.48
1:C:3204:ALA:O	1:C:3207:ILE:HG22	2.13	0.48
1:C:3011:LEU:HD22	1:C:3096:ILE:HG12	1.94	0.48
1:C:3025:VAL:HG22	1:C:3037:ILE:HD13	1.95	0.48
1:C:3176:SER:O	1:C:3180:ASN:HB2	2.13	0.48
1:A:1229:LYS:NZ	1:A:1229:LYS:HB3	2.28	0.48
1:C:3184:VAL:HG22	1:C:3189:VAL:HG23	1.96	0.48
1:D:4237:LEU:N	1:D:4237:LEU:HD12	2.29	0.48
1:D:4008:ILE:HG23	1:D:4119:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4050:VAL:O	1:D:4054:ARG:HG3	2.14	0.48
1:A:1073:ASP:HB2	1:A:1103:ASN:ND2	2.28	0.48
1:A:1100:TYR:HB3	1:A:1108:LEU:HG	1.95	0.48
1:D:4237:LEU:HD11	3:D:5106:HOH:O	2.13	0.48
1:A:1108:LEU:C	1:A:1108:LEU:HD12	2.34	0.48
1:A:1241:GLU:O	1:A:1245:VAL:HG23	2.14	0.47
1:B:2061:ASN:ND2	1:B:2072:GLY:HA3	2.29	0.47
1:C:3047:ARG:NH1	1:C:3048:MET:HG2	2.29	0.47
1:D:4004:LEU:O	1:D:4008:ILE:HG13	2.15	0.47
1:C:3003:ARG:CB	1:C:3108:LEU:HD21	2.44	0.47
1:C:3163:ARG:HH12	1:C:3248:GLU:HB2	1.80	0.47
1:C:3154:VAL:O	1:C:3155:ASP:HB2	2.14	0.47
1:D:4209:VAL:HG21	1:D:4233:PHE:HD2	1.79	0.47
1:B:2044:GLU:HG3	1:B:2047:ARG:NH2	2.29	0.47
1:A:1194:THR:HG23	1:A:1194:THR:O	2.15	0.47
1:B:2163:ARG:HD3	1:B:2163:ARG:O	2.15	0.47
1:D:4242:VAL:O	1:D:4246:VAL:HG23	2.15	0.47
1:B:2143:LEU:HG	1:B:2168:THR:HG22	1.97	0.47
1:B:2253:ILE:HG22	1:B:2254:GLY:N	2.29	0.47
1:C:3247:ASN:N	1:C:3247:ASN:HD22	2.12	0.46
1:C:3140:ASN:OD1	1:D:4030:LYS:HE3	2.15	0.46
1:D:4039:THR:HG22	1:D:4043:ARG:CZ	2.45	0.46
1:C:3121:TYR:CZ	1:C:3129:PHE:HB2	2.50	0.46
1:A:1027:ASN:HB3	1:A:1040:GLU:OE2	2.15	0.46
1:B:2025:VAL:HG11	1:B:2039:THR:HG21	1.96	0.46
1:B:2227:PHE:HA	1:B:2231:PHE:HZ	1.79	0.46
1:C:3121:TYR:CE2	1:C:3129:PHE:HB2	2.51	0.46
1:C:3241:GLU:O	1:C:3245:VAL:HG23	2.16	0.46
1:C:3156:PHE:HA	1:C:3253:ILE:HD11	1.98	0.46
1:A:1112:HIS:O	1:A:1114:PRO:HD3	2.15	0.46
1:A:1199:PRO:HG3	1:A:1228:SER:O	2.15	0.46
1:D:4148:GLY:HA3	1:D:4191:PHE:CZ	2.50	0.46
1:A:1160:PHE:HA	1:A:1249:VAL:HG21	1.98	0.46
1:D:4036:ASP:O	1:D:4040:GLU:HG3	2.16	0.46
1:A:1155:ASP:O	1:A:1159:LYS:HD2	2.17	0.45
1:A:1061:ASN:HB3	1:A:1070:GLU:HB2	1.98	0.45
1:B:2247:ASN:CA	1:B:2250:VAL:HG12	2.46	0.45
1:D:4054:ARG:HG2	1:D:4054:ARG:NH2	2.31	0.45
1:D:4191:PHE:HA	1:D:4233:PHE:O	2.16	0.45
1:D:4176:SER:O	1:D:4180:ASN:HB2	2.17	0.45
1:A:1031:LYS:CG	1:A:1032:THR:H	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:ILE:HG23	1:A:1119:THR:HG21	1.98	0.45
1:B:2030:LYS:HD3	1:B:2034:PHE:HA	1.97	0.45
1:C:3105:GLU:HB2	1:C:3107:LYS:HE3	1.98	0.45
1:D:4137:VAL:HG11	1:D:4214:GLY:HA3	1.97	0.45
1:A:1153:TYR:HB2	1:A:1156:PHE:HB3	1.99	0.45
1:B:2219:PHE:CG	1:B:2230:ASN:HB2	2.51	0.45
1:C:3164:MET:HB3	1:C:3171:ILE:HD11	1.99	0.45
1:D:4170:ARG:HG3	1:D:4172:ARG:NH1	2.32	0.45
1:B:2163:ARG:HD3	1:B:2163:ARG:C	2.36	0.44
1:A:1062:ILE:HG22	1:A:1063:MET:N	2.32	0.44
1:A:1020:ILE:HD11	1:D:4017:LEU:HA	1.99	0.44
1:C:3028:VAL:O	1:C:3032:THR:HG22	2.17	0.44
1:C:3045:ALA:HB3	1:C:3080:PRO:HB3	1.99	0.44
1:D:4011:LEU:HD22	1:D:4096:ILE:CG2	2.48	0.44
1:D:4123:GLU:HB2	1:D:4126:SER:HB2	2.00	0.44
1:B:2106:VAL:HG13	1:B:2106:VAL:O	2.17	0.44
1:B:2130:PHE:HB2	1:B:2135:ILE:HG21	1.99	0.44
1:B:2195:TRP:O	1:B:2196:ARG:O	2.36	0.44
1:D:4014:VAL:HA	1:D:4048:MET:HE3	1.98	0.44
1:C:3146:CYS:O	1:C:3169:ARG:HB3	2.18	0.44
1:D:4076:TRP:CE3	1:D:4098:LEU:HD21	2.53	0.44
1:B:2092:PRO:HB2	1:B:2116:LEU:HD21	2.00	0.43
1:B:2241:GLU:OE1	1:B:2241:GLU:N	2.49	0.43
1:D:4037:ILE:O	1:D:4041:ILE:HG12	2.18	0.43
1:B:2176:SER:O	1:B:2180:ASN:HB2	2.19	0.43
1:C:3047:ARG:HD3	1:C:3048:MET:N	2.33	0.43
1:C:3191:PHE:HA	1:C:3233:PHE:O	2.19	0.43
1:C:3062:ILE:O	1:C:3065:GLU:HG3	2.18	0.43
1:D:4146:CYS:O	1:D:4169:ARG:HB3	2.17	0.43
1:A:1197:ILE:C	1:A:1197:ILE:HD12	2.38	0.43
1:B:2244:LYS:O	1:B:2248:GLU:HG3	2.18	0.43
1:D:4222:LYS:O	1:D:4223:GLU:C	2.57	0.43
1:A:1066:GLU:O	1:A:1066:GLU:HG2	2.19	0.43
1:B:2029:GLU:CD	1:B:2043:ARG:HH22	2.22	0.43
1:A:1086:ASN:HD21	1:A:1175:GLY:HA3	1.84	0.43
1:B:2153:TYR:CD2	1:B:2195:TRP:HB3	2.53	0.43
1:C:3004:LEU:O	1:C:3008:ILE:HG13	2.19	0.43
1:D:4164:MET:HG3	1:D:4168:THR:CG2	2.48	0.43
1:A:1121:TYR:CZ	1:A:1129:PHE:HB2	2.54	0.43
1:C:3089:HIS:O	1:D:4188:ARG:HA	2.19	0.43
1:A:1244:LYS:HB2	1:A:1244:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4130:PHE:HB2	1:D:4135:ILE:HG21	2.01	0.43
1:D:4098:LEU:HD23	1:D:4098:LEU:C	2.38	0.43
1:D:4164:MET:HG3	1:D:4168:THR:HG21	2.01	0.42
1:A:1225:ASN:ND2	1:A:1227:PHE:H	2.17	0.42
1:A:1151:GLY:HA3	1:A:1153:TYR:CZ	2.55	0.42
1:B:2146:CYS:O	1:B:2169:ARG:HB3	2.19	0.42
1:D:4250:VAL:HA	1:D:4253:ILE:HD12	2.00	0.42
1:A:1061:ASN:OD1	1:A:1072:GLY:HA3	2.20	0.42
1:D:4197:ILE:HG13	1:D:4197:ILE:O	2.19	0.42
1:B:2021:HIS:CD2	1:B:2041:ILE:HD12	2.55	0.42
1:B:2146:CYS:SG	1:B:2238:ILE:HD13	2.60	0.42
1:D:4159:LYS:O	1:D:4162:GLU:HB2	2.20	0.42
1:A:1218:ASP:C	1:A:1220:SER:H	2.22	0.42
1:C:3092:PRO:HB2	1:C:3116:LEU:HD21	2.01	0.42
1:D:4025:VAL:O	1:D:4025:VAL:HG12	2.20	0.42
1:A:1030:LYS:H	1:A:1030:LYS:HG3	1.51	0.42
1:A:1031:LYS:O	1:A:1033:GLY:N	2.53	0.42
1:A:1124:GLU:N	1:A:1207:ILE:HD11	2.35	0.42
1:C:3253:ILE:HG22	1:C:3254:GLY:N	2.34	0.42
1:D:4195:TRP:HA	1:D:4230:ASN:OD1	2.19	0.42
1:D:4238:ILE:C	1:D:4238:ILE:HD12	2.40	0.42
1:B:2003:ARG:HB3	1:B:2108:LEU:HD21	2.01	0.41
1:B:2120:LEU:HD12	1:B:2120:LEU:N	2.35	0.41
1:D:4035:LYS:HB3	1:D:4035:LYS:NZ	2.35	0.41
1:C:3102:GLU:CB	1:C:3107:LYS:HD3	2.49	0.41
1:D:4054:ARG:CZ	1:D:4062:ILE:HD12	2.50	0.41
1:C:3120:LEU:HD22	1:C:3182:ALA:HB1	2.01	0.41
1:A:1017:LEU:HA	1:D:4020:ILE:HD11	2.02	0.41
1:A:1108:LEU:HA	1:A:1207:ILE:HD13	2.02	0.41
1:A:1219:PHE:CE2	1:A:1230:ASN:HB2	2.55	0.41
1:B:2197:ILE:HG13	1:B:2198:ASN:N	2.35	0.41
1:A:1040:GLU:HG2	1:A:1041:ILE:HD13	2.03	0.41
1:A:1194:THR:CG2	1:A:1231:PHE:HB2	2.50	0.41
1:B:2038:VAL:HG22	1:B:2039:THR:N	2.35	0.41
1:B:2105:GLU:H	1:B:2105:GLU:HG3	1.65	0.41
1:B:2244:LYS:HB3	1:B:2244:LYS:NZ	2.35	0.41
1:D:4053:ILE:HD12	1:D:4078:ILE:HD11	2.01	0.41
1:A:1046:GLN:O	1:A:1050:VAL:HG23	2.19	0.41
1:A:1148:GLY:HA3	1:A:1191:PHE:CE1	2.55	0.41
1:C:3112:HIS:O	1:C:3114:PRO:HD3	2.21	0.41
1:C:3148:GLY:HA3	1:C:3191:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2130:PHE:CD1	1:B:2130:PHE:C	2.95	0.41
1:B:2239:HIS:O	1:B:2243:VAL:HG23	2.21	0.41
1:D:4014:VAL:HG13	1:D:4048:MET:CE	2.51	0.41
1:D:4142:SER:OG	1:D:4145:GLU:HG3	2.20	0.41
1:D:4184:VAL:CG2	1:D:4189:VAL:HG23	2.49	0.41
1:D:4124:GLU:HA	1:D:4211:GLU:OE2	2.21	0.41
1:A:1031:LYS:HB2	1:A:1038:VAL:HB	2.03	0.41
1:A:1044:GLU:HG2	1:A:1047:ARG:HH22	1.85	0.41
1:A:1089:HIS:CD2	1:B:2147:VAL:HG21	2.56	0.41
1:D:4166:LYS:H	1:D:4166:LYS:HG3	1.68	0.41
1:D:4028:VAL:HG23	1:D:4029:GLU:HG2	2.02	0.40
1:D:4017:LEU:HD22	1:D:4048:MET:HE1	2.03	0.40
1:D:4134:ARG:HB3	1:D:4134:ARG:CZ	2.50	0.40
1:C:3194:THR:OG1	1:C:3231:PHE:HB2	2.21	0.40
1:C:3046:GLN:O	1:C:3050:VAL:HG23	2.22	0.40
1:B:2001:MET:HG3	1:B:2123:GLU:OE1	2.21	0.40
1:C:3239:HIS:O	1:C:3243:VAL:HG23	2.21	0.40
1:D:4147:VAL:HA	1:D:4170:ARG:O	2.21	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	252/256 (98%)	236 (94%)	13 (5%)	3 (1%)	13	19
1	B	252/256 (98%)	230 (91%)	19 (8%)	3 (1%)	13	19
1	C	252/256 (98%)	240 (95%)	9 (4%)	3 (1%)	13	19
1	D	252/256 (98%)	231 (92%)	20 (8%)	1 (0%)	34	48
All	All	1008/1024 (98%)	937 (93%)	61 (6%)	10 (1%)	15	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1032	THR
1	C	3253	ILE
1	D	4026	ASP
1	A	1034	PHE
1	A	1196	ARG
1	B	2228	SER
1	B	2196	ARG
1	B	2253	ILE
1	C	3169	ARG
1	C	3163	ARG

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	212/213 (100%)	202 (95%)	10 (5%)	26 42
1	B	212/213 (100%)	203 (96%)	9 (4%)	30 47
1	C	212/213 (100%)	208 (98%)	4 (2%)	57 75
1	D	212/213 (100%)	204 (96%)	8 (4%)	33 51
All	All	848/852 (100%)	817 (96%)	31 (4%)	34 53

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1026	ASP
1	A	1030	LYS
1	A	1036	ASP
1	A	1043	ARG
1	A	1066	GLU
1	A	1124	GLU
1	A	1130	PHE
1	A	1167	ARG
1	A	1180	ASN
1	A	1244	LYS
1	B	2066	GLU
1	B	2069	PHE

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Mol	Chain	Res	Type
1	B	2105	GLU
1	B	2130	PHE
1	B	2163	ARG
1	B	2180	ASN
1	B	2196	ARG
1	B	2230	ASN
1	B	2244	LYS
1	C	3047	ARG
1	C	3107	LYS
1	C	3206	LEU
1	C	3230	ASN
1	D	4071	LYS
1	D	4073	ASP
1	D	4130	PHE
1	D	4165	GLU
1	D	4166	LYS
1	D	4167	ARG
1	D	4180	ASN
1	D	4229	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1021	HIS
1	A	1046	GLN
1	A	1093	ASN
1	A	1103	ASN
1	A	1180	ASN
1	A	1225	ASN
1	B	2021	HIS
1	B	2061	ASN
1	B	2103	ASN
1	B	2140	ASN
1	B	2180	ASN
1	B	2198	ASN
1	B	2230	ASN
1	B	2247	ASN
1	C	3093	ASN
1	C	3247	ASN
1	D	4021	HIS
1	D	4061	ASN
1	D	4103	ASN

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Mol	Chain	Res	Type
1	D	4140	ASN
1	D	4180	ASN
1	D	4247	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

4 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	SRT	B	4501	-	3,9,9	1.97	1 (33%)	6,12,12	1.97	2 (33%)
2	SRT	D	4503	-	3,9,9	1.98	1 (33%)	6,12,12	2.00	2 (33%)
2	SRT	C	4504	-	3,9,9	2.02	1 (33%)	6,12,12	2.03	2 (33%)
2	SRT	B	4502	-	3,9,9	2.14	1 (33%)	6,12,12	1.85	2 (33%)

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	SRT	B	4501	-	2/2/4/4	0/4/12/12	-
2	SRT	D	4503	-	2/2/4/4	0/4/12/12	-
2	SRT	C	4504	-	2/2/4/4	0/4/12/12	-
2	SRT	B	4502	-	2/2/4/4	0/4/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4502	SRT	O3-C3	3.19	1.48	1.42
2	B	4501	SRT	O3-C3	2.94	1.48	1.42
2	D	4503	SRT	O3-C3	2.90	1.48	1.42
2	C	4504	SRT	O3-C3	2.82	1.48	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4504	SRT	O2-C2-C1	-3.56	102.54	111.10
2	D	4503	SRT	O2-C2-C1	-3.30	103.17	111.10
2	B	4501	SRT	O2-C2-C1	-3.13	103.58	111.10
2	B	4502	SRT	C4-C3-C2	-2.94	106.78	113.11
2	D	4503	SRT	C4-C3-C2	-2.85	106.97	113.11
2	B	4501	SRT	C4-C3-C2	-2.84	106.99	113.11
2	B	4502	SRT	O2-C2-C1	-2.67	104.66	111.10
2	C	4504	SRT	C4-C3-C2	-2.31	108.13	113.11

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	4501	SRT	C2
2	B	4501	SRT	C3
2	D	4503	SRT	C2
2	D	4503	SRT	C3
2	C	4504	SRT	C2
2	C	4504	SRT	C3
2	B	4502	SRT	C2
2	B	4502	SRT	C3

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	254/256 (99%)	-0.30	11 (4%) 35 33	16, 33, 81, 133	0
1	B	254/256 (99%)	-0.16	10 (3%) 39 38	18, 33, 74, 110	0
1	C	254/256 (99%)	-0.48	1 (0%) 92 91	15, 30, 66, 83	0
1	D	254/256 (99%)	0.08	22 (8%) 10 9	17, 38, 125, 151	0
All	All	1016/1024 (99%)	-0.22	44 (4%) 35 33	15, 33, 81, 151	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4028	VAL	11.8
1	D	4032	THR	7.1
1	B	2227	PHE	6.5
1	A	1253	ILE	5.8
1	D	4027	ASN	5.8
1	D	4069	PHE	5.6
1	D	4026	ASP	5.0
1	D	4066	GLU	4.8
1	D	4030	LYS	4.7
1	D	4068	ILE	4.6
1	D	4029	GLU	4.3
1	A	1032	THR	4.2
1	D	4033	GLY	4.2
1	D	4031	LYS	4.1
1	B	2001	MET	3.9
1	D	4065	GLU	3.9
1	A	1031	LYS	3.5
1	A	1027	ASN	3.1
1	B	2250	VAL	2.9
1	B	2197	ILE	2.8
1	A	1034	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	4253	ILE	2.7
1	D	4059	ASP	2.7
1	A	1250	VAL	2.6
1	D	4001	MET	2.6
1	C	3001	MET	2.6
1	A	1254	GLY	2.5
1	B	2226	ALA	2.5
1	D	4025	VAL	2.5
1	B	2200	TRP	2.5
1	B	2244	LYS	2.5
1	B	2228	SER	2.4
1	D	4074	ARG	2.3
1	D	4067	GLY	2.3
1	D	4252	GLU	2.3
1	B	2199	PRO	2.2
1	A	1251	GLU	2.2
1	D	4070	GLU	2.2
1	A	1195	TRP	2.2
1	D	4037	ILE	2.1
1	A	1001	MET	2.1
1	D	4071	LYS	2.1
1	A	1033	GLY	2.1
1	B	2163	ARG	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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SRT	B	4502	10/10	0.67	0.29	53,59,61,65	0
2	SRT	B	4501	10/10	0.75	0.20	53,58,60,62	0
2	SRT	D	4503	10/10	0.81	0.17	42,49,52,57	0
2	SRT	C	4504	10/10	0.82	0.18	51,54,57,59	0

6.5 Other polymers (i)

There are no such residues in this entry.