Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 11:26 PM EST

PDB ID	:	1P4D
Title	:	F factor TraI Relaxase Domain
Authors	:	Datta, S.; Larkin, C.; Schildbach, J.F.
Deposited on	:	2003-04-22
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

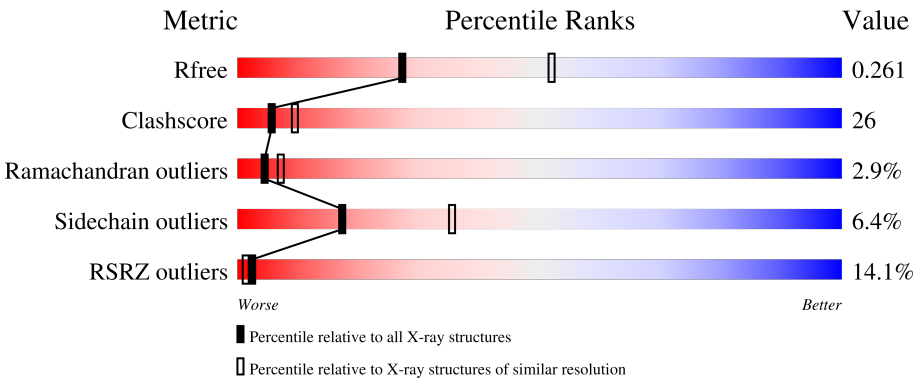
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	330	5%; 55%; 23%; 5%; 17%
1	B	330	5%; 57%; 24%; •; 16%
1	C	330	25%; 36%; 42%; 5%; 16%

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	EDO	B	607	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6656 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.

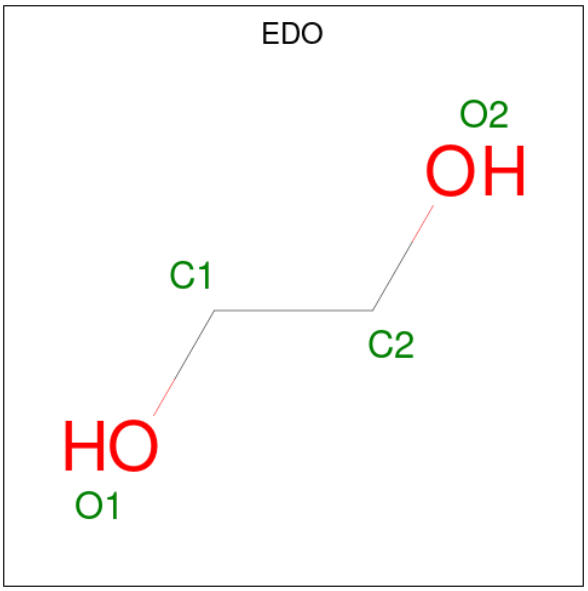
- Molecule 1 is a protein called TraI protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2149	1331	387	418	13	0	1	0
1	B	276	2148	1331	386	418	13	0	0	0
1	C	276	2148	1331	386	418	13	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	81	83	83	0	2

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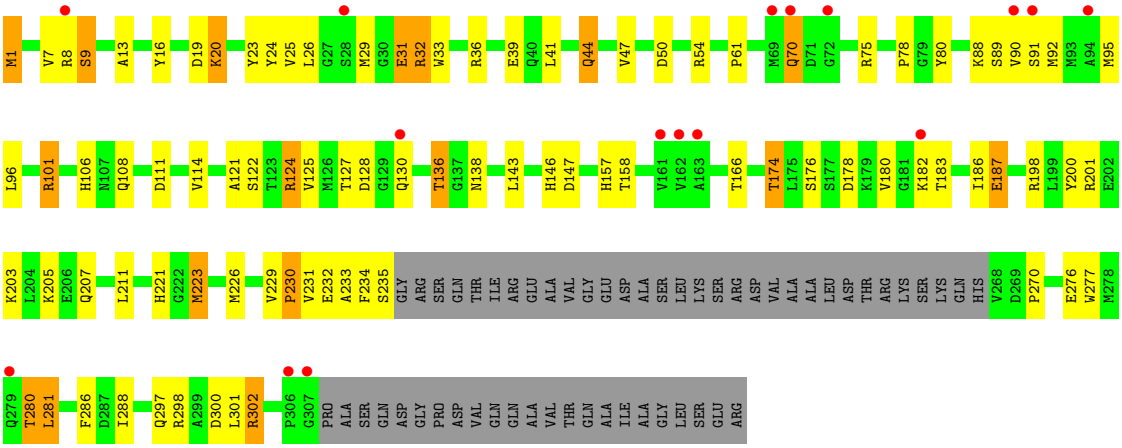
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	72	72	72	0	0
			Total	O		
4	C	9	9	9	0	0

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.

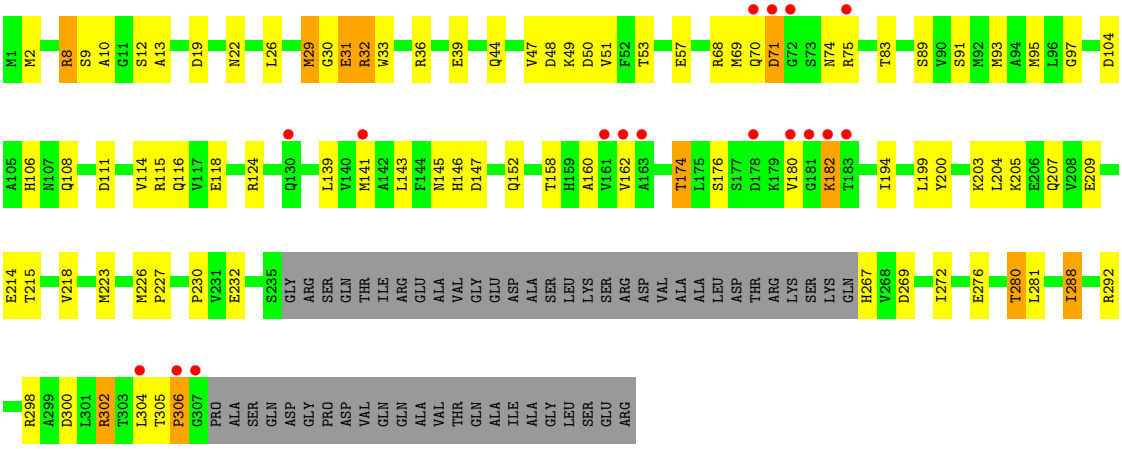
• Molecule 1: TraI protein

Chain A:



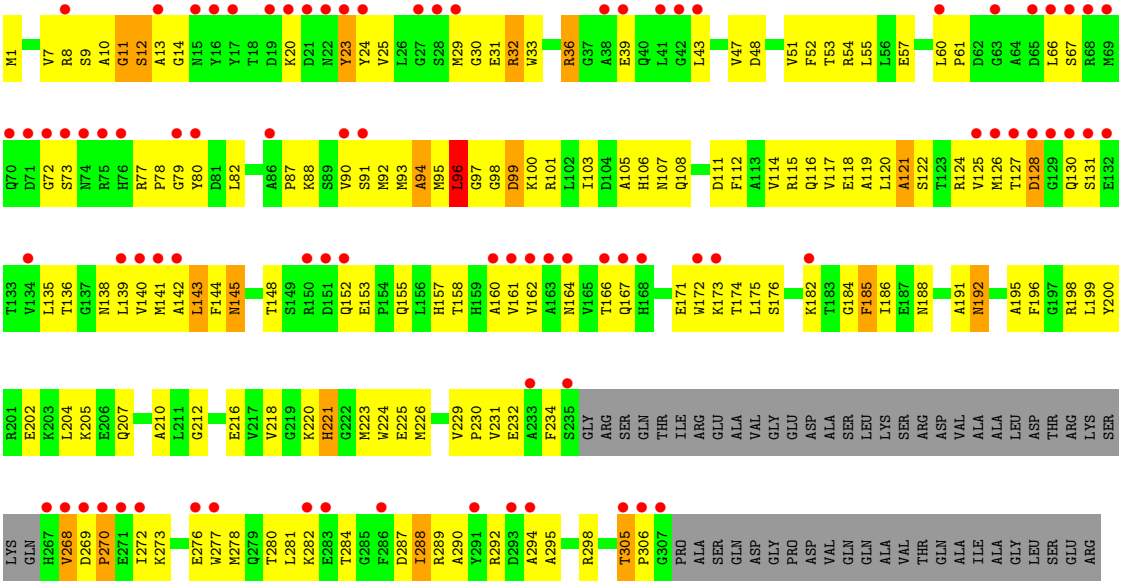
• Molecule 1: TraI protein

Chain B:



• Molecule 1: TraI protein

Chain C:


M1 V7 R8 S9 A10 G11 S12 A13 G14 N15 Y16 Y17 T18 D19 K20 D21 N22 Y23 Y24 V25 L26 G27 S28 M29 G30 E31 R32 W33 R36 G37 A38 E39 Q40 L41 G42 L43 V47 D48 V51 F52 T53 R54 L55 L56 E57 L60 P61 D62 G63 A64 D65 L66 S67 R68 M69
Q70 D71 G72 S73 N74 R75 H76 R77 P78 G79 Y80 D81 L82 A86 P87 K88 S89 V90 S91 M92 M93 A94 M95 L96 G97 G98 D99 K100 R101 L102 I103 D104 A105 H106 N107 Q108 D111 F112 A113 V114 R115 Q116 V117 E118 A119 L120 A121 S122 T123 R124 V125 M126 T127 D128 G129 Q130 S131 E132
T133 V134 L135 T136 G137 N138 L139 V140 M141 A142 L143 F144 N145 T148 S149 R150 D151 Q152 E153 P154 Q155 L156 H157 T158 H159 A160 V161 V162 A163 N164 V165 T166 Q167 H168 E171 W172 K173 T174 L175 S176 K182 T183 G184 F185 I186 E187 N188 A191 N192 A195 F196 G197 R198 L199 Y200
R201 E202 K203 L204 K205 E206 Q207 A210 L211 G212 E216 V217 V218 G219 K220 H221 G222 M223 W224 E225 M226 V229 P230 V231 E232 A233 F234 S235 GLY ARG SER GLN THR ILE ARG GLU ALA VAL GLY GLU ASP ALA SER LEU LYS SER ARG ASP VAL ALA ALA LEU ASP THR ARG LYS SER
LYS GLN H267 V268 D269 P270 E271 I272 K273 E276 W277 M278 G279 T280 L281 K282 E283 T284 G285 F286 D287 I288 R289 A290 Y291 R292 D293 A294 A295 R298 T305 P306 G307 PRO ALA SER GLN GLY PRO ASP VAL GLN GLN ALA VAL THR GLN ALA ILE ALA GLY LEU SER GLU ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.22Å 128.22Å 121.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.60 24.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.9 (25.00-2.60) 96.2 (24.93-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.44 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.278 0.220 , 0.261	Depositor DCC
R_{free} test set	3441 reflections (8.56%)	wwPDB-VP
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 64.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6656	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: MG, EDO

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	0.42	0/2187	0.66	0/2950
1	B	0.39	0/2187	0.61	0/2951
1	C	0.28	0/2187	0.52	0/2951
All	All	0.37	0/6561	0.60	0/8852

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 (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	2149	0	2086	85	0
1	B	2148	0	2081	84	0
1	C	2148	0	2081	162	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	20	0	30	3	0
3	B	20	0	30	0	0
3	C	4	0	6	0	0
4	A	83	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	72	0	0	0	0
4	C	9	0	0	2	0
All	All	6656	0	6314	328	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 26.

All (328) 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:8:ARG:HH11	1:B:8:ARG:H	1.12	0.98
1:A:136:THR:HG21	1:A:166:THR:OG1	1.63	0.98
1:B:305:THR:HB	1:B:306:PRO:HD2	1.45	0.95
1:A:198:ARG:HD2	1:A:201:ARG:HH11	1.39	0.87
1:C:33:TRP:HE1	1:C:47:VAL:HA	1.41	0.86
1:C:268:VAL:HG12	1:C:269:ASP:H	1.40	0.85
1:B:269:ASP:HB3	1:B:272:ILE:HG12	1.59	0.83
1:A:29:MET:CE	1:A:31:GLU:HG2	2.10	0.81
1:A:88:LYS:HG3	1:A:92:MET:HE2	1.62	0.80
1:B:8:ARG:HG2	1:B:9:SER:H	1.46	0.79
1:A:101:ARG:NH1	1:A:211:LEU:HD22	1.98	0.79
1:B:8:ARG:HG2	1:B:9:SER:N	1.98	0.79
1:A:111:ASP:HA	3:A:612:EDO:H21	1.64	0.78
1:C:33:TRP:CZ2	1:C:47:VAL:HG13	2.19	0.77
1:C:66:LEU:HD11	1:C:172:TRP:O	1.85	0.77
1:C:97:GLY:O	1:C:288:ILE:HD11	1.86	0.76
1:A:8:ARG:HD3	1:A:16:TYR:CE2	2.21	0.76
1:A:44:GLN:HA	1:A:44:GLN:HE21	1.52	0.74
1:B:116:GLN:HG3	1:B:199:LEU:HD13	1.70	0.74
1:B:39:GLU:HG3	1:B:44:GLN:NE2	2.04	0.72
1:A:124:ARG:HH12	1:A:182:LYS:HB2	1.53	0.72
1:B:8:ARG:HH11	1:B:8:ARG:N	1.87	0.72
1:C:192:ASN:N	1:C:192:ASN:HD22	1.88	0.72
1:A:276:GLU:O	1:A:280:THR:HG22	1.89	0.72
1:A:207:GLN:HB3	3:A:600:EDO:H22	1.72	0.71
1:A:7:VAL:CG1	1:A:78:PRO:HB2	2.21	0.71
1:B:305:THR:HB	1:B:306:PRO:CD	2.17	0.71
1:B:49:LYS:O	1:B:53:THR:HG23	1.91	0.70
1:C:29:MET:CE	1:C:31:GLU:HG2	2.21	0.70
1:A:174:THR:HG22	1:A:176:SER:O	1.91	0.70
1:C:20:LYS:HG2	1:C:23:TYR:OH	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HG2	1:A:231:VAL:HG13	1.75	0.69
1:C:171:GLU:HB2	1:C:173:LYS:HE3	1.74	0.68
1:B:269:ASP:HB3	1:B:272:ILE:CG1	2.22	0.68
1:C:33:TRP:NE1	1:C:47:VAL:HA	2.08	0.68
1:C:88:LYS:HZ1	1:C:234:PHE:HB3	1.58	0.68
1:A:29:MET:HE2	1:A:31:GLU:HG2	1.77	0.67
1:C:98:GLY:O	1:C:100:LYS:HG3	1.93	0.67
1:B:106:HIS:HD2	1:B:200:TYR:OH	1.78	0.67
1:B:174:THR:HG22	1:B:176:SER:O	1.94	0.67
1:C:148:THR:CG2	1:C:152:GLN:HA	2.25	0.67
1:A:91:SER:O	1:A:95:MET:HG2	1.95	0.66
1:C:91:SER:O	1:C:95:MET:HG2	1.93	0.66
1:C:198:ARG:HD2	1:C:221:HIS:HB3	1.76	0.66
1:A:8:ARG:O	1:A:13:ALA:HB2	1.96	0.66
1:B:194:ILE:N	1:B:194:ILE:HD12	2.11	0.65
1:C:136:THR:HG21	1:C:166:THR:OG1	1.97	0.65
1:C:204:LEU:HD12	1:C:224:TRP:CZ2	2.32	0.65
1:A:223:MET:HG2	4:A:940:HOH:O	1.97	0.65
1:C:88:LYS:NZ	1:C:234:PHE:HB3	2.12	0.65
1:A:89:SER:HA	1:A:92:MET:HE3	1.79	0.64
1:C:144:PHE:C	1:C:145:ASN:HD22	2.01	0.64
1:A:198:ARG:HD2	1:A:201:ARG:NH1	2.10	0.64
1:C:52:PHE:HZ	1:C:161:VAL:HG11	1.63	0.64
1:A:198:ARG:HD3	1:A:221:HIS:HB3	1.80	0.64
1:B:8:ARG:HD3	1:B:13:ALA:HA	1.80	0.64
1:A:136:THR:CG2	1:A:166:THR:OG1	2.40	0.64
1:C:57:GLU:O	1:C:67:SER:HB3	1.97	0.64
1:A:281:LEU:HD11	1:A:288:ILE:HD11	1.79	0.63
1:A:20:LYS:HA	1:A:23:TYR:CE2	2.33	0.63
1:B:93:MET:HE3	1:B:97:GLY:HA3	1.80	0.63
1:B:288:ILE:C	1:B:288:ILE:HD13	2.19	0.63
1:B:232:GLU:H	1:B:232:GLU:CD	2.01	0.62
1:B:194:ILE:HD12	1:B:194:ILE:H	1.64	0.62
1:C:145:ASN:HD22	1:C:145:ASN:N	1.98	0.62
1:A:124:ARG:NH1	1:A:182:LYS:HB2	2.14	0.62
1:C:268:VAL:HG12	1:C:269:ASP:N	2.15	0.61
1:A:174:THR:CG2	1:A:176:SER:O	2.48	0.61
1:C:48:ASP:OD2	1:C:51:VAL:HG23	2.00	0.61
1:A:114:VAL:HG12	3:A:612:EDO:H12	1.81	0.61
1:A:92:MET:HE1	1:A:229:VAL:HG12	1.82	0.61
1:B:70:GLN:HG2	1:B:75:ARG:NH1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:THR:O	1:C:128:ASP:HB2	2.01	0.60
1:C:148:THR:HG23	1:C:152:GLN:HA	1.83	0.60
1:C:305:THR:HB	1:C:306:PRO:CD	2.31	0.60
1:C:77:ARG:HB2	1:C:164:ASN:ND2	2.17	0.60
1:B:8:ARG:HD3	1:B:13:ALA:CA	2.32	0.60
1:C:82:LEU:HB2	1:C:160:ALA:HB3	1.84	0.60
1:C:280:THR:O	1:C:284:THR:HG23	2.02	0.59
1:C:29:MET:HE2	1:C:31:GLU:HG2	1.82	0.59
1:A:50:ASP:HB3	1:A:54:ARG:HH21	1.67	0.59
1:B:70:GLN:O	1:B:71:ASP:HB2	2.03	0.59
1:C:29:MET:HG2	1:C:31:GLU:HB3	1.84	0.59
1:B:298:ARG:O	1:B:302:ARG:HG2	2.04	0.58
1:C:54:ARG:NH1	1:C:61:PRO:HA	2.19	0.58
1:A:26:LEU:HG	1:A:147:ASP:HB3	1.84	0.58
1:C:87:PRO:HG2	1:C:90:VAL:CG2	2.34	0.58
1:B:269:ASP:CB	1:B:272:ILE:HG12	2.33	0.57
1:B:29:MET:HB3	1:B:31:GLU:HG3	1.85	0.57
1:B:106:HIS:CD2	1:B:200:TYR:OH	2.57	0.57
1:B:2:MET:HA	1:B:83:THR:O	2.05	0.57
1:A:127:THR:O	1:A:130:GLN:HG2	2.05	0.57
1:C:95:MET:C	1:C:97:GLY:H	2.08	0.56
1:B:124:ARG:HH22	1:B:182:LYS:HB2	1.70	0.56
1:A:29:MET:HE3	1:A:31:GLU:HG2	1.84	0.56
1:C:130:GLN:O	1:C:130:GLN:HG3	2.06	0.56
1:C:92:MET:O	1:C:95:MET:O	2.24	0.56
1:B:29:MET:SD	1:B:31:GLU:HG2	2.45	0.56
1:B:104:ASP:O	1:B:108:GLN:HG3	2.06	0.56
1:B:124:ARG:NH2	1:B:182:LYS:HB2	2.20	0.56
1:C:25:VAL:HG21	1:C:277:TRP:HZ3	1.71	0.55
1:A:20:LYS:HA	1:A:23:TYR:CZ	2.41	0.55
1:C:127:THR:O	1:C:130:GLN:HG2	2.07	0.55
1:C:288:ILE:HD13	1:C:288:ILE:C	2.27	0.55
1:A:24:TYR:CD2	1:A:270:PRO:HB2	2.41	0.55
1:C:80:TYR:HE1	1:C:185:PHE:HD2	1.53	0.55
1:A:106:HIS:HD2	1:A:200:TYR:OH	1.89	0.55
1:C:292:ARG:O	1:C:295:ALA:HB3	2.07	0.55
1:C:204:LEU:HD13	1:C:204:LEU:O	2.06	0.55
1:A:50:ASP:HB3	1:A:54:ARG:NH2	2.22	0.55
1:C:20:LYS:HA	1:C:23:TYR:CZ	2.42	0.54
1:C:33:TRP:CD1	1:C:47:VAL:HG22	2.43	0.54
1:A:7:VAL:HG13	1:A:78:PRO:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:TRP:CZ3	1:C:43:LEU:HD13	2.42	0.54
1:C:53:THR:O	1:C:57:GLU:HG3	2.08	0.54
1:C:218:VAL:HG12	1:C:218:VAL:O	2.08	0.54
1:C:8:ARG:O	1:C:13:ALA:HB2	2.08	0.54
1:C:139:LEU:HB2	1:C:141:MET:HE2	1.90	0.54
1:C:288:ILE:HG23	1:C:289:ARG:N	2.22	0.54
1:B:108:GLN:HB2	1:B:207:GLN:HE22	1.72	0.53
1:C:144:PHE:O	1:C:158:THR:HA	2.08	0.53
1:B:8:ARG:H	1:B:8:ARG:NH1	1.94	0.53
1:C:30:GLY:O	1:C:32:ARG:HG3	2.09	0.53
1:C:204:LEU:HD12	1:C:224:TRP:CH2	2.44	0.53
1:C:184:GLY:O	1:C:188:ASN:ND2	2.41	0.53
1:A:80:TYR:CD2	1:A:186:ILE:HD12	2.43	0.53
1:C:220:LYS:O	1:C:223:MET:HG3	2.09	0.53
1:B:93:MET:HB2	1:B:226:MET:HE1	1.90	0.52
1:A:183:THR:HA	1:A:187:GLU:OE1	2.10	0.52
1:B:302:ARG:O	1:B:305:THR:HG23	2.09	0.52
1:C:95:MET:O	1:C:97:GLY:N	2.42	0.52
1:C:278:MET:O	1:C:282:LYS:HG3	2.10	0.52
1:B:143:LEU:CD2	1:B:160:ALA:HA	2.40	0.52
1:C:29:MET:HE3	1:C:31:GLU:HG2	1.90	0.52
1:C:96:LEU:C	1:C:96:LEU:HD12	2.30	0.52
1:C:80:TYR:CD1	1:C:186:ILE:HD13	2.45	0.52
1:A:70:GLN:HB3	1:A:75:ARG:HG3	1.91	0.51
1:B:93:MET:HB2	1:B:226:MET:CE	2.40	0.51
1:B:91:SER:HB3	1:B:95:MET:CE	2.41	0.51
1:C:9:SER:O	1:C:11:GLY:N	2.43	0.51
1:C:52:PHE:O	1:C:55:LEU:HB3	2.11	0.51
1:B:30:GLY:O	1:B:32:ARG:HD2	2.11	0.51
1:A:92:MET:O	1:A:96:LEU:HB2	2.11	0.51
1:B:89:SER:HB2	1:B:226:MET:HE2	1.93	0.51
1:C:195:ALA:O	1:C:198:ARG:HB2	2.10	0.51
1:C:210:ALA:C	1:C:212:GLY:H	2.13	0.51
1:B:194:ILE:H	1:B:194:ILE:CD1	2.24	0.51
1:C:25:VAL:HG12	1:C:95:MET:HB2	1.93	0.51
1:C:33:TRP:NE1	1:C:47:VAL:HG22	2.26	0.50
1:B:8:ARG:H	1:B:8:ARG:HD2	1.75	0.50
1:C:88:LYS:HG3	1:C:92:MET:HE2	1.93	0.50
1:C:270:PRO:O	1:C:273:LYS:HB3	2.10	0.50
1:A:122:SER:HA	1:A:136:THR:HB	1.92	0.50
1:A:25:VAL:HG21	1:A:277:TRP:HZ3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:VAL:HA	1:C:226:MET:CE	2.42	0.50
1:C:138:ASN:O	1:C:139:LEU:HG	2.11	0.50
1:C:202:GLU:O	1:C:205:LYS:HB3	2.11	0.50
1:A:25:VAL:HG21	1:A:277:TRP:CZ3	2.47	0.50
1:C:55:LEU:HD21	1:C:140:VAL:CG1	2.42	0.50
1:A:108:GLN:OE1	1:A:207:GLN:NE2	2.44	0.50
1:A:234:PHE:O	1:A:235:SER:HB3	2.12	0.50
1:C:112:PHE:O	1:C:116:GLN:HG2	2.12	0.50
1:C:114:VAL:HG13	1:C:141:MET:SD	2.52	0.50
1:A:136:THR:HG23	1:A:138:ASN:ND2	2.27	0.49
1:B:22:ASN:HB3	1:B:146:HIS:CD2	2.47	0.49
1:C:108:GLN:HB2	1:C:207:GLN:HE22	1.76	0.49
1:A:88:LYS:HG3	1:A:92:MET:CE	2.38	0.49
1:B:91:SER:HB3	1:B:95:MET:HE1	1.92	0.49
1:C:93:MET:CE	1:C:93:MET:HA	2.42	0.49
1:A:300:ASP:CG	1:B:36:ARG:HH22	2.15	0.49
1:B:218:VAL:HG12	1:B:223:MET:CE	2.42	0.49
1:C:96:LEU:HD13	1:C:281:LEU:HD12	1.93	0.49
1:A:41:LEU:HD13	1:A:61:PRO:HD2	1.93	0.49
1:A:286:PHE:HD1	1:A:288:ILE:HD12	1.76	0.49
1:C:278:MET:HB3	1:C:282:LYS:HE3	1.95	0.49
1:A:298:ARG:O	1:A:302:ARG:HG3	2.13	0.49
1:B:19:ASP:HB3	1:B:22:ASN:ND2	2.28	0.49
1:B:33:TRP:CZ2	1:B:47:VAL:HG13	2.48	0.49
1:A:1:MET:HB3	1:A:201:ARG:HH21	1.78	0.49
1:C:164:ASN:OD1	1:C:174:THR:HG23	2.13	0.49
1:A:1:MET:HB3	1:A:201:ARG:NH2	2.28	0.49
1:B:69:MET:SD	1:B:74:ASN:HB2	2.53	0.48
1:C:204:LEU:HD12	1:C:224:TRP:HZ2	1.77	0.48
1:A:92:MET:CE	1:A:231:VAL:HG22	2.43	0.48
1:B:68:ARG:O	1:B:75:ARG:HG2	2.14	0.48
1:B:300:ASP:O	1:B:304:LEU:HG	2.13	0.48
1:C:287:ASP:HB3	1:C:290:ALA:HB3	1.96	0.48
1:A:90:VAL:HA	1:A:226:MET:HE1	1.95	0.48
1:C:281:LEU:HD23	1:C:281:LEU:O	2.14	0.48
1:A:54:ARG:HD2	4:A:957:HOH:O	2.12	0.48
1:C:124:ARG:HH22	1:C:182:LYS:HB2	1.78	0.48
1:A:8:ARG:HD3	1:A:16:TYR:CZ	2.49	0.48
1:B:10:ALA:CB	1:B:57:GLU:HG3	2.44	0.48
1:A:125:VAL:HG13	1:A:125:VAL:O	2.14	0.47
1:C:77:ARG:O	1:C:164:ASN:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LYS:HB3	1:C:103:ILE:HD12	1.95	0.47
1:C:23:TYR:HB3	1:C:145:ASN:O	2.12	0.47
1:C:191:ALA:C	1:C:192:ASN:HD22	2.17	0.47
1:C:80:TYR:HE1	1:C:185:PHE:CD2	2.31	0.47
1:C:107:ASN:HA	4:C:910:HOH:O	2.13	0.47
1:C:126:MET:HA	1:C:131:SER:HA	1.96	0.47
1:A:229:VAL:HA	1:A:230:PRO:HD3	1.71	0.47
1:C:161:VAL:HG12	4:C:906:HOH:O	2.14	0.47
1:C:294:ALA:O	1:C:298:ARG:HB2	2.14	0.47
1:B:218:VAL:HG12	1:B:223:MET:HE2	1.96	0.47
1:C:23:TYR:CD2	1:C:29:MET:HB2	2.50	0.47
1:C:60:LEU:HB3	1:C:61:PRO:HD2	1.96	0.47
1:C:117:VAL:HG22	1:C:196:PHE:CE1	2.49	0.47
1:C:142:ALA:O	1:C:144:PHE:CE1	2.68	0.47
1:B:32:ARG:NH2	1:B:111:ASP:OD1	2.47	0.47
1:C:95:MET:C	1:C:97:GLY:N	2.69	0.46
1:C:185:PHE:O	1:C:188:ASN:N	2.47	0.46
1:A:297:GLN:O	1:A:301:LEU:HB2	2.15	0.46
1:C:55:LEU:HD21	1:C:140:VAL:HG12	1.97	0.46
1:C:192:ASN:N	1:C:192:ASN:ND2	2.58	0.46
1:C:164:ASN:ND2	1:C:174:THR:HG23	2.30	0.46
1:B:205:LYS:O	1:B:209:GLU:HG3	2.14	0.46
1:B:8:ARG:CG	1:B:9:SER:H	2.24	0.46
1:B:48:ASP:OD2	1:B:51:VAL:HG23	2.15	0.46
1:A:286:PHE:CD1	1:A:288:ILE:HD12	2.51	0.46
1:C:87:PRO:HB2	1:C:225:GLU:OE1	2.15	0.45
1:C:29:MET:HG2	1:C:31:GLU:CB	2.46	0.45
1:A:95:MET:SD	1:A:147:ASP:HB2	2.57	0.45
1:B:302:ARG:HG2	1:B:302:ARG:H	1.61	0.45
1:C:174:THR:HG22	1:C:176:SER:N	2.31	0.45
1:C:92:MET:CE	1:C:231:VAL:HA	2.46	0.45
1:A:32:ARG:HD2	1:A:143:LEU:HB2	1.98	0.45
1:A:39:GLU:OE2	1:B:292:ARG:NH1	2.49	0.45
1:B:174:THR:CG2	1:B:176:SER:O	2.62	0.45
1:C:7:VAL:HG23	1:C:80:TYR:C	2.37	0.45
1:B:143:LEU:HD22	1:B:160:ALA:HA	1.98	0.45
1:B:145:ASN:ND2	1:B:158:THR:OG1	2.50	0.45
1:A:92:MET:HE2	1:A:231:VAL:HA	1.97	0.45
1:B:33:TRP:CE2	1:B:47:VAL:HG22	2.52	0.45
1:A:31:GLU:H	1:A:31:GLU:HG3	1.59	0.45
1:A:106:HIS:HE1	1:A:158:THR:OG1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:THR:HB	1:C:306:PRO:HD3	1.98	0.45
1:A:32:ARG:NE	1:A:143:LEU:HD12	2.32	0.45
1:B:118:GLU:HA	1:B:139:LEU:CD1	2.47	0.44
1:C:118:GLU:HA	1:C:139:LEU:CD1	2.47	0.44
1:C:141:MET:HG2	1:C:162:VAL:HA	1.99	0.44
1:A:33:TRP:CE2	1:A:47:VAL:HG22	2.52	0.44
1:A:232:GLU:HG2	1:A:233:ALA:N	2.32	0.44
1:C:210:ALA:C	1:C:212:GLY:N	2.70	0.44
4:A:969:HOH:O	1:B:115:ARG:HD2	2.18	0.44
1:C:25:VAL:HG21	1:C:277:TRP:CZ3	2.52	0.44
1:C:51:VAL:C	1:C:54:ARG:HG2	2.38	0.44
1:C:155:GLN:O	1:C:157:HIS:ND1	2.51	0.44
1:A:174:THR:HG23	1:A:176:SER:N	2.32	0.44
1:A:300:ASP:OD2	1:B:36:ARG:NH2	2.50	0.44
1:C:23:TYR:CG	1:C:29:MET:HB2	2.53	0.44
1:C:36:ARG:HB2	1:C:138:ASN:CB	2.47	0.44
1:C:36:ARG:O	1:C:39:GLU:HB3	2.18	0.44
1:C:111:ASP:O	1:C:115:ARG:HG3	2.17	0.44
1:A:8:ARG:NH1	1:A:16:TYR:CE1	2.86	0.44
1:C:106:HIS:HE1	1:C:158:THR:OG1	2.01	0.44
1:C:268:VAL:HG12	1:C:272:ILE:HG13	1.99	0.44
1:A:127:THR:O	1:A:128:ASP:HB2	2.18	0.44
1:B:276:GLU:O	1:B:280:THR:HG22	2.17	0.44
1:C:116:GLN:O	1:C:119:ALA:HB3	2.18	0.44
1:C:220:LYS:N	1:C:223:MET:HE2	2.33	0.44
1:B:114:VAL:HG13	1:B:141:MET:CE	2.47	0.43
1:C:9:SER:C	1:C:11:GLY:N	2.72	0.43
1:C:277:TRP:O	1:C:280:THR:HG22	2.18	0.43
1:A:88:LYS:CG	1:A:231:VAL:HG13	2.48	0.43
1:C:174:THR:CG2	1:C:176:SER:H	2.32	0.43
1:B:214:GLU:O	1:B:227:PRO:HD3	2.18	0.43
1:C:25:VAL:CG1	1:C:95:MET:HB2	2.49	0.43
1:C:229:VAL:O	1:C:231:VAL:HG23	2.18	0.43
1:A:92:MET:CE	1:A:231:VAL:HA	2.49	0.43
1:B:174:THR:HG23	1:B:176:SER:H	1.84	0.43
1:C:120:LEU:O	1:C:121:ALA:C	2.56	0.43
1:C:12:SER:C	1:C:14:GLY:H	2.21	0.43
1:C:72:GLY:O	1:C:73:SER:HB3	2.19	0.43
1:C:269:ASP:HB3	1:C:272:ILE:HG12	2.01	0.43
1:C:276:GLU:O	1:C:280:THR:HG22	2.19	0.43
1:C:127:THR:O	1:C:128:ASP:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:THR:CG2	1:C:175:LEU:N	2.82	0.42
1:B:10:ALA:HB1	1:B:57:GLU:HG3	2.00	0.42
1:B:141:MET:HG2	1:B:162:VAL:HG22	2.01	0.42
1:C:125:VAL:O	1:C:125:VAL:HG13	2.17	0.42
1:C:216:GLU:O	1:C:218:VAL:HG23	2.19	0.42
1:B:205:LYS:HD2	1:B:215:THR:OG1	2.19	0.42
1:A:203:LYS:O	1:A:207:GLN:HG2	2.19	0.42
1:B:48:ASP:OD2	1:B:50:ASP:HB2	2.19	0.42
1:B:124:ARG:HH22	1:B:182:LYS:CG	2.32	0.42
1:C:54:ARG:HE	1:C:54:ARG:HB2	1.63	0.42
1:C:51:VAL:O	1:C:54:ARG:HG2	2.19	0.42
1:C:145:ASN:N	1:C:145:ASN:ND2	2.66	0.42
1:C:288:ILE:HG23	1:C:289:ARG:HG3	2.02	0.42
1:C:164:ASN:HD21	1:C:174:THR:HG23	1.85	0.42
1:A:201:ARG:NE	4:A:939:HOH:O	2.48	0.42
1:B:8:ARG:HG3	1:B:12:SER:OG	2.20	0.42
1:B:26:LEU:HG	1:B:147:ASP:HB3	2.02	0.42
1:C:166:THR:HG23	1:C:167:GLN:N	2.34	0.42
1:B:12:SER:O	1:B:13:ALA:C	2.58	0.41
1:B:70:GLN:O	1:B:71:ASP:CB	2.68	0.41
1:C:143:LEU:N	1:C:143:LEU:HD23	2.35	0.41
1:A:146:HIS:HB2	1:A:157:HIS:NE2	2.35	0.41
1:A:198:ARG:CD	1:A:221:HIS:O	2.68	0.41
1:B:152:GLN:HE21	1:B:152:GLN:HB3	1.53	0.41
1:C:11:GLY:O	1:C:13:ALA:N	2.53	0.41
1:C:80:TYR:CG	1:C:186:ILE:HD13	2.56	0.41
1:C:96:LEU:HD13	1:C:281:LEU:CD1	2.50	0.41
1:C:204:LEU:HD13	1:C:204:LEU:C	2.40	0.41
1:A:8:ARG:O	1:A:9:SER:C	2.59	0.41
1:B:108:GLN:CB	1:B:207:GLN:HE22	2.34	0.41
1:C:36:ARG:HB2	1:C:138:ASN:HB2	2.02	0.41
1:C:94:ALA:HA	1:C:99:ASP:O	2.20	0.41
1:B:124:ARG:HH22	1:B:182:LYS:CB	2.33	0.41
1:C:122:SER:HB3	1:C:135:LEU:HA	2.02	0.41
1:C:139:LEU:HD12	1:C:141:MET:HE1	2.03	0.41
1:C:164:ASN:HD21	1:C:174:THR:CG2	2.33	0.41
1:C:23:TYR:CE2	1:C:29:MET:SD	3.13	0.41
1:C:36:ARG:HD3	1:C:36:ARG:H	1.86	0.41
1:C:105:ALA:HA	1:C:207:GLN:NE2	2.35	0.41
1:B:124:ARG:HH22	1:B:182:LYS:HD2	1.86	0.41
1:C:7:VAL:HG23	1:C:79:GLY:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:HIS:HA	1:C:204:LEU:HD23	2.04	0.40
1:C:268:VAL:CG1	1:C:269:ASP:N	2.81	0.40
1:C:272:ILE:HG22	1:C:276:GLU:OE1	2.22	0.40
1:A:121:ALA:CB	1:A:136:THR:HG22	2.51	0.40
1:B:93:MET:CE	1:B:288:ILE:HG12	2.52	0.40
1:C:148:THR:HA	1:C:153:GLU:O	2.21	0.40
1:A:121:ALA:HB1	1:A:136:THR:HG22	2.03	0.40
1:A:198:ARG:HD3	1:A:221:HIS:O	2.21	0.40
1:C:99:ASP:OD1	1:C:101:ARG:HB2	2.22	0.40
1:C:118:GLU:HA	1:C:139:LEU:HD12	2.03	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	272/330 (82%)	256 (94%)	13 (5%)	3 (1%)	14 30
1	B	272/330 (82%)	251 (92%)	16 (6%)	5 (2%)	8 16
1	C	272/330 (82%)	217 (80%)	39 (14%)	16 (6%)	1 1
All	All	816/990 (82%)	724 (89%)	68 (8%)	24 (3%)	4 7

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	C	96	LEU
1	B	180	VAL
1	B	306	PRO
1	C	10	ALA
1	C	94	ALA
1	C	99	ASP

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Mol	Chain	Res	Type
1	C	121	ALA
1	C	221	HIS
1	C	305	THR
1	B	71	ASP
1	B	182	LYS
1	C	12	SER
1	C	11	GLY
1	C	185	PHE
1	A	20	LYS
1	C	23	TYR
1	C	24	TYR
1	C	78	PRO
1	C	128	ASP
1	A	230	PRO
1	B	230	PRO
1	C	230	PRO
1	C	268	VAL

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	225/267 (84%)	206 (92%)	19 (8%)	11	21
1	B	225/267 (84%)	213 (95%)	12 (5%)	22	45
1	C	225/267 (84%)	213 (95%)	12 (5%)	22	45
All	All	675/801 (84%)	632 (94%)	43 (6%)	17	35

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	ASP
1	A	31	GLU
1	A	32	ARG
1	A	36	ARG

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Mol	Chain	Res	Type
1	A	44	GLN
1	A	70	GLN
1	A	101	ARG
1	A	124	ARG
1	A	136	THR
1	A	174	THR
1	A	178	ASP
1	A	180	VAL
1	A	187	GLU
1	A	205	LYS
1	A	223	MET
1	A	280	THR
1	A	281	LEU
1	A	302	ARG
1	B	8	ARG
1	B	29	MET
1	B	31	GLU
1	B	32	ARG
1	B	174	THR
1	B	203	LYS
1	B	204	LEU
1	B	267	HIS
1	B	280	THR
1	B	281	LEU
1	B	288	ILE
1	B	302	ARG
1	C	1	MET
1	C	32	ARG
1	C	36	ARG
1	C	96	LEU
1	C	143	LEU
1	C	145	ASN
1	C	192	ASN
1	C	199	LEU
1	C	200	TYR
1	C	232	GLU
1	C	270	PRO
1	C	288	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	44	GLN
1	A	70	GLN
1	A	76	HIS
1	A	106	HIS
1	A	107	ASN
1	A	130	GLN
1	A	145	ASN
1	A	152	GLN
1	A	297	GLN
1	B	6	GLN
1	B	22	ASN
1	B	70	GLN
1	B	106	HIS
1	B	107	ASN
1	B	130	GLN
1	B	145	ASN
1	B	152	GLN
1	B	207	GLN
1	B	297	GLN
1	C	6	GLN
1	C	22	ASN
1	C	70	GLN
1	C	106	HIS
1	C	107	ASN
1	C	130	GLN
1	C	138	ASN
1	C	145	ASN
1	C	146	HIS
1	C	152	GLN
1	C	169	ASN
1	C	188	ASN
1	C	192	ASN
1	C	207	GLN
1	C	297	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

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	$\#\|Z\| > 2$
3	EDO	B	604	-	3,3,3	0.62	0	2,2,2	0.20	0
3	EDO	A	612	-	3,3,3	0.67	0	2,2,2	0.11	0
3	EDO	B	605	-	3,3,3	0.64	0	2,2,2	0.17	0
3	EDO	B	602	-	3,3,3	0.67	0	2,2,2	0.17	0
3	EDO	A	608	-	3,3,3	0.65	0	2,2,2	0.20	0
3	EDO	C	603	-	3,3,3	0.64	0	2,2,2	0.13	0
3	EDO	B	607	-	3,3,3	0.62	0	2,2,2	0.21	0
3	EDO	B	610	-	3,3,3	0.64	0	2,2,2	0.23	0
3	EDO	A	601	-	3,3,3	0.63	0	2,2,2	0.22	0
3	EDO	A	606	-	3,3,3	0.70	0	2,2,2	0.16	0
3	EDO	A	600	-	3,3,3	0.62	0	2,2,2	0.09	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
3	EDO	B	604	-	-	1/1/1/1	-
3	EDO	A	612	-	-	1/1/1/1	-
3	EDO	B	605	-	-	1/1/1/1	-
3	EDO	B	602	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	608	-	-	1/1/1/1	-
3	EDO	C	603	-	-	1/1/1/1	-
3	EDO	B	607	-	-	1/1/1/1	-
3	EDO	B	610	-	-	1/1/1/1	-
3	EDO	A	601	-	-	1/1/1/1	-
3	EDO	A	606	-	-	1/1/1/1	-
3	EDO	A	600	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	EDO	O1-C1-C2-O2
3	A	601	EDO	O1-C1-C2-O2
3	A	606	EDO	O1-C1-C2-O2
3	A	608	EDO	O1-C1-C2-O2
3	A	612	EDO	O1-C1-C2-O2
3	B	602	EDO	O1-C1-C2-O2
3	B	604	EDO	O1-C1-C2-O2
3	B	605	EDO	O1-C1-C2-O2
3	B	607	EDO	O1-C1-C2-O2
3	B	610	EDO	O1-C1-C2-O2
3	C	603	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	612	EDO	2	0
3	A	600	EDO	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	275/330 (83%)	0.03	16 (5%)	23	17	26, 45, 73, 104	0
1	B	276/330 (83%)	0.13	17 (6%)	20	15	29, 49, 84, 116	0
1	C	276/330 (83%)	1.57	84 (30%)	0	0	56, 105, 152, 161	0
All	All	827/990 (83%)	0.57	117 (14%)	2	1	26, 59, 139, 161	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	GLY	9.9
1	C	268	VAL	8.7
1	C	134	VAL	8.5
1	C	307	GLY	8.0
1	B	306	PRO	7.6
1	C	127	THR	7.0
1	C	267	HIS	6.9
1	C	24	TYR	6.6
1	C	306	PRO	6.6
1	C	22	ASN	6.5
1	C	129	GLY	6.3
1	C	70	GLN	6.2
1	C	272	ILE	6.1
1	C	73	SER	6.1
1	C	71	ASP	6.1
1	A	307	GLY	6.0
1	C	128	ASP	5.9
1	C	75	ARG	5.8
1	B	180	VAL	5.7
1	C	72	GLY	5.6
1	C	126	MET	5.6
1	C	23	TYR	5.5
1	C	69	MET	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	74	ASN	5.1
1	C	269	ASP	5.1
1	C	29	MET	5.0
1	A	306	PRO	5.0
1	C	125	VAL	4.8
1	C	150	ARG	4.7
1	C	20	LYS	4.7
1	C	131	SER	4.7
1	C	66	LEU	4.5
1	C	63	GLY	4.5
1	C	15	ASN	4.4
1	C	28	SER	4.3
1	C	151	ASP	4.3
1	C	161	VAL	4.3
1	C	166	THR	4.3
1	C	163	ALA	4.2
1	C	130	GLN	4.2
1	B	181	GLY	4.1
1	C	172	TRP	4.1
1	C	152	GLN	4.0
1	C	167	GLN	4.0
1	C	282	LYS	4.0
1	C	162	VAL	4.0
1	C	132	GLU	3.9
1	C	141	MET	3.9
1	B	182	LYS	3.9
1	C	42	GLY	3.9
1	C	271	GLU	3.8
1	C	21	ASP	3.7
1	C	182	LYS	3.6
1	B	72	GLY	3.5
1	B	75	ARG	3.5
1	A	72	GLY	3.4
1	C	140	VAL	3.4
1	C	173	LYS	3.4
1	C	39	GLU	3.3
1	C	235	SER	3.3
1	A	182	LYS	3.2
1	B	162	VAL	3.2
1	B	163	ALA	3.2
1	C	41	LEU	3.2
1	A	69	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	16	TYR	3.1
1	C	142	ALA	3.0
1	C	76	HIS	3.0
1	C	65	ASP	2.9
1	C	91	SER	2.9
1	C	291	TYR	2.8
1	C	233	ALA	2.8
1	C	80	TYR	2.7
1	C	305	THR	2.7
1	B	70	GLN	2.7
1	C	283	GLU	2.7
1	C	60	LEU	2.7
1	A	161	VAL	2.6
1	C	17	TYR	2.6
1	C	293	ASP	2.6
1	C	8	ARG	2.6
1	C	160	ALA	2.6
1	B	183	THR	2.5
1	A	162	VAL	2.5
1	C	276	GLU	2.5
1	C	286	PHE	2.5
1	C	68	ARG	2.4
1	C	90	VAL	2.4
1	B	130	GLN	2.4
1	C	270	PRO	2.4
1	A	163	ALA	2.4
1	C	294	ALA	2.4
1	A	94	ALA	2.3
1	C	13	ALA	2.3
1	B	71	ASP	2.3
1	C	79	GLY	2.2
1	C	139	LEU	2.2
1	A	91	SER	2.2
1	A	130	GLN	2.2
1	C	38	ALA	2.2
1	A	279	GLN	2.2
1	C	19	ASP	2.2
1	A	90	VAL	2.2
1	B	178	ASP	2.1
1	C	27	GLY	2.1
1	C	168	HIS	2.1
1	C	86	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	28	SER	2.1
1	B	141	MET	2.1
1	A	70	GLN	2.0
1	A	8	ARG	2.0
1	C	67	SER	2.0
1	C	277	TRP	2.0
1	B	304	LEU	2.0
1	B	161	VAL	2.0
1	C	164	ASN	2.0
1	C	43	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, 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	B-factors(Å^2)	Q<0.9
3	EDO	B	607	4/4	0.52	0.41	114,114,114,115	0
3	EDO	B	602	4/4	0.74	0.20	74,76,77,79	0
3	EDO	A	608	4/4	0.78	0.18	75,78,78,78	0
3	EDO	C	603	4/4	0.83	0.38	89,89,89,90	0
3	EDO	A	606	4/4	0.87	0.24	76,78,78,79	0
3	EDO	B	610	4/4	0.88	0.45	84,84,85,85	0
3	EDO	A	612	4/4	0.90	0.35	57,59,59,61	0
3	EDO	A	600	4/4	0.91	0.30	63,64,65,65	0
3	EDO	B	605	4/4	0.92	0.43	68,69,70,70	0
2	MG	B	901	1/1	0.93	0.28	52,52,52,52	0
3	EDO	A	601	4/4	0.93	0.18	84,85,86,87	0
3	EDO	B	604	4/4	0.94	0.44	86,86,86,86	0
2	MG	C	902	1/1	0.95	0.31	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	900	1/1	0.99	0.09	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.