



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:27 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

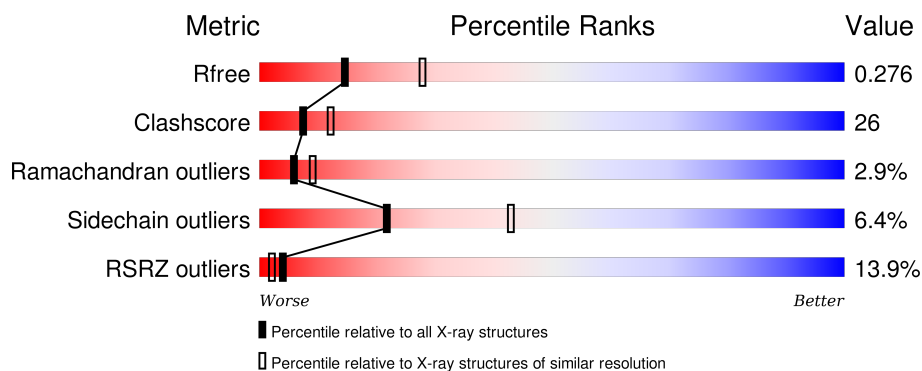
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	<div> <div>5%</div> <div>55% 23% 5% 17%</div> </div>
1	B	330	<div> <div>5%</div> <div>57% 24% • 16%</div> </div>
1	C	330	<div> <div>25%</div> <div>36% 42% 5% 16%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	600	-	-	-	X
3	EDO	A	612	-	-	-	X
3	EDO	B	605	-	-	-	X
3	EDO	B	610	-	-	-	X
3	EDO	C	603	-	-	-	X

2 Entry composition

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
1	A	275	Total	C	N	O	S	0	1	0
			2149	1331	387	418	13			
1	B	276	Total	C	N	O	S	0	0	0
			2148	1331	386	418	13			
1	C	276	Total	C	N	O	S	0	0	0
			2148	1331	386	418	13			

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

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is water.

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

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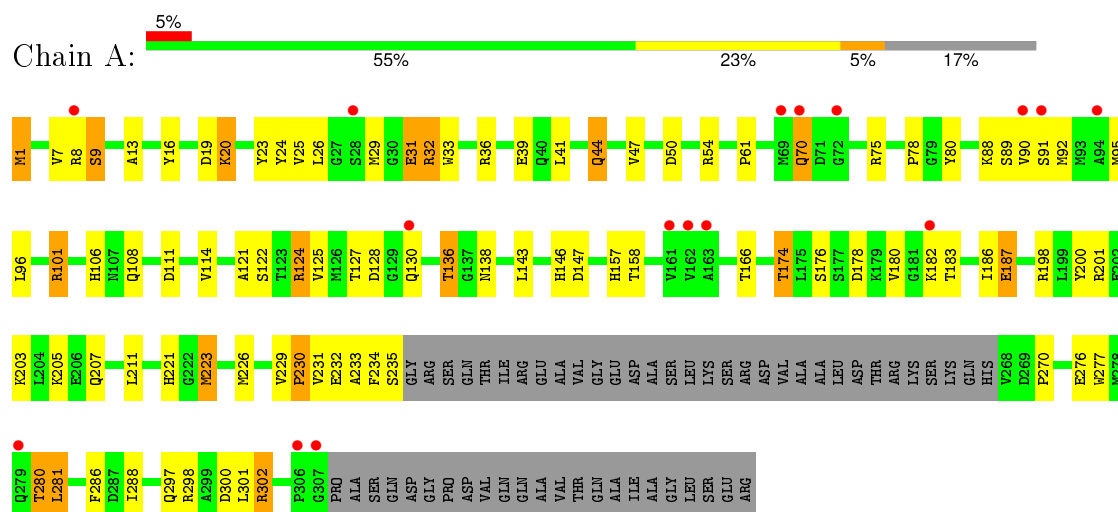
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	72	Total	O	0	0
			72	72		
4	C	9	Total	O	0	0
			9	9		

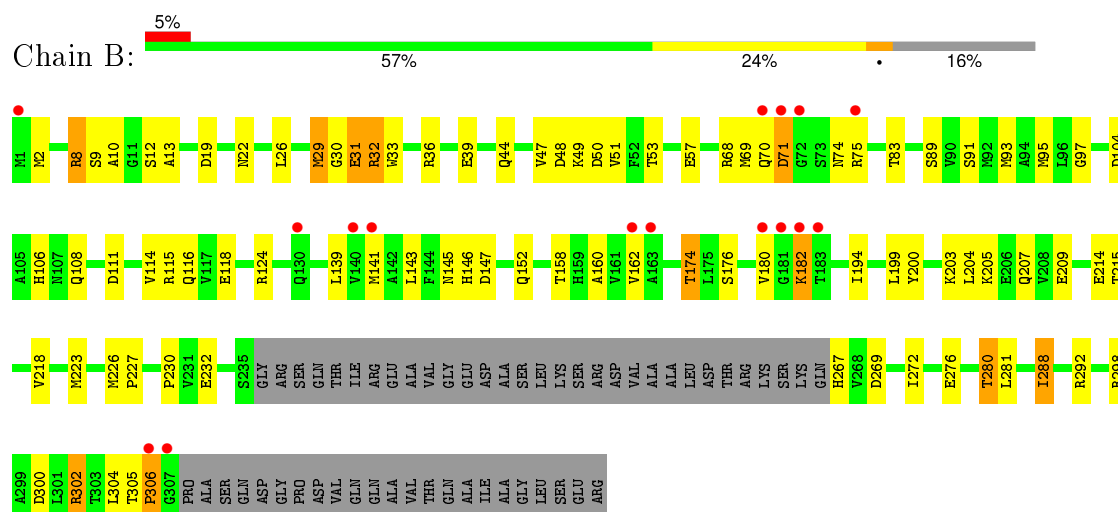
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: TraI protein

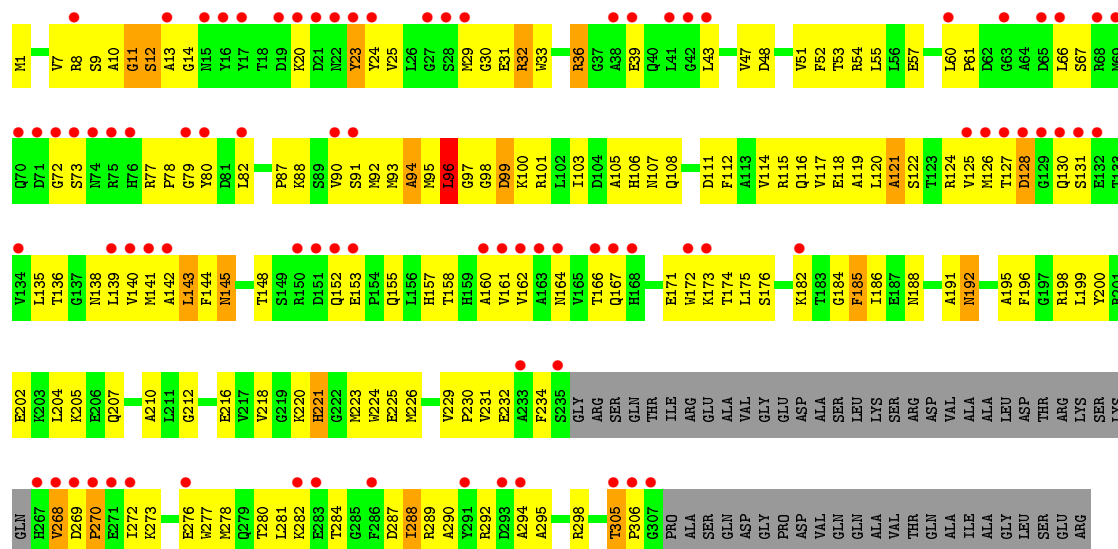


• Molecule 1: TraI protein



• Molecule 1: TraI protein





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.278 0.233 , 0.276	Depositor DCC
R_{free} test set	3441 reflections (9.93%)	DCC
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 , 64.5	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 40186 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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:H	1:B:8:ARG:HH11	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:B:8:ARG:HG2	1:B:9:SER:N	1.98	0.79
1:A:101:ARG:NH1	1:A:211:LEU:HD22	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:B:305:THR:HB	1:B:306:PRO:CD	2.17	0.71
1:A:7:VAL:CG1	1:A:78:PRO:HB2	2.21	0.71
1:C:29:MET:CE	1:C:31:GLU:HG2	2.21	0.70
1:B:49:LYS:O	1:B:53:THR:HG23	1.91	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:HD12	1:B:194:ILE:N	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:C:88:LYS:NZ	1:C:234:PHE:HB3	2.12	0.65
1:A:223:MET:HG2	4:A:940:HOH:O	1.97	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:CD	1:B:232:GLU:H	2.01	0.62
1:C:145:ASN:HD22	1:C:145:ASN:N	1.98	0.62
1:B:194:ILE:HD12	1:B:194:ILE:H	1.64	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:B:70:GLN:O	1:B:71:ASP:HB2	2.03	0.59
1:A:50:ASP:HB3	1:A:54:ARG:HH21	1.67	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:106:HIS:CD2	1:B:200:TYR:OH	2.57	0.57
1:B:29:MET:HB3	1:B:31:GLU:HG3	1.85	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:HG3	1:C:130:GLN:O	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:124:ARG:NH2	1:B:182:LYS:HB2	2.20	0.56
1:B:104:ASP:O	1:B:108:GLN:HG3	2.06	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:C:292:ARG:O	1:C:295:ALA:HB3	2.07	0.55
1:A:106:HIS:HD2	1:A:200:TYR:OH	1.89	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:C:33:TRP:CZ3	1:C:43:LEU:HD13	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG13	1:A:78:PRO:HB2	1.88	0.54
1:C:53:THR:O	1:C:57:GLU:HG3	2.08	0.54
1:C:218:VAL:O	1:C:218:VAL:HG12	2.08	0.54
1:C:139:LEU:HB2	1:C:141:MET:HE2	1.90	0.54
1:C:8:ARG:O	1:C:13:ALA:HB2	2.08	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: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:A:183:THR:HA	1:A:187:GLU:OE1	2.10	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:B:93:MET:HB2	1:B:226:MET:CE	2.40	0.51
1:A:70:GLN:HB3	1:A:75:ARG:HG3	1.91	0.51
1:C:9:SER:O	1:C:11:GLY:N	2.43	0.51
1:B:91:SER:HB3	1:B:95:MET:CE	2.41	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:C:195:ALA:O	1:C:198:ARG:HB2	2.10	0.51
1:B:89:SER:HB2	1:B:226:MET:HE2	1.93	0.51
1:C:210:ALA:C	1:C:212:GLY:H	2.13	0.51
1:C:25:VAL:HG12	1:C:95:MET:HB2	1.93	0.51
1:B:194:ILE:H	1:B:194:ILE:CD1	2.24	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:C:90:VAL:HA	1:C:226:MET:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASN:O	1:C:139:LEU:HG	2.11	0.50
1:A:25:VAL:HG21	1:A:277:TRP:HZ3	1.76	0.50
1:C:202:GLU:O	1:C:205:LYS:HB3	2.11	0.50
1:C:55:LEU:HD21	1:C:140:VAL:CG1	2.42	0.50
1:A:25:VAL:HG21	1:A:277:TRP:CZ3	2.47	0.50
1:A:108:GLN:OE1	1:A:207:GLN:NE2	2.44	0.50
1:C:114:VAL:HG13	1:C:141:MET:SD	2.52	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:A:136:THR:HG23	1:A:138:ASN:ND2	2.27	0.49
1:C:108:GLN:HB2	1:C:207:GLN:HE22	1.76	0.49
1:B:22:ASN:HB3	1:B:146:HIS:CD2	2.47	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:C:96:LEU:HD13	1:C:281:LEU:HD12	1.93	0.49
1:B:218:VAL:HG12	1:B:223:MET:CE	2.42	0.49
1:A:300:ASP:CG	1:B:36:ARG:HH22	2.15	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: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:298:ARG:O	1:A:302:ARG:HG3	2.13	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:C:100:LYS:HB3	1:C:103:ILE:HD12	1.95	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:A:125:VAL:O	1:A:125:VAL:HG13	2.14	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:142:ALA:O	1:C:144:PHE:CE1	2.68	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: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:192:ASN:N	1:C:192:ASN:ND2	2.58	0.46
1:C:55:LEU:HD21	1:C:140:VAL:HG12	1.97	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:B:302:ARG:H	1:B:302:ARG:HG2	1.61	0.45
1:A:95:MET:SD	1:A:147:ASP:HB2	2.57	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: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: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: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:HG3	1:A:31:GLU:H	1.59	0.45
1:C:305:THR:HB	1:C:306:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:HIS:HE1	1:A:158:THR:OG1	2.00	0.45
1:A:32:ARG:NE	1:A:143:LEU:HD12	2.32	0.45
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:B:118:GLU:HA	1:B:139:LEU:CD1	2.47	0.44
1:C:210:ALA:C	1:C:212:GLY:N	2.70	0.44
1:A:232:GLU:HG2	1:A:233:ALA:N	2.32	0.44
1:A:33:TRP:CE2	1:A:47:VAL:HG22	2.52	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:C:23:TYR:CG	1:C:29:MET:HB2	2.53	0.44
1:A:174:THR:HG23	1:A:176:SER:N	2.32	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:A:300:ASP:OD2	1:B:36:ARG:NH2	2.50	0.44
1:C:111:ASP:O	1:C:115:ARG:HG3	2.17	0.44
1:C:268:VAL:HG12	1:C:272:ILE:HG13	1.99	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:A:127:THR:O	1:A:128:ASP:HB2	2.18	0.44
1:C:220:LYS:N	1:C:223:MET:HE2	2.33	0.44
1:C:116:GLN:O	1:C:119:ALA:HB3	2.18	0.44
1:B:276:GLU:O	1:B:280:THR:HG22	2.17	0.44
1:C:9:SER:C	1:C:11:GLY:N	2.72	0.43
1:B:114:VAL:HG13	1:B:141:MET:CE	2.47	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:C:25:VAL:CG1	1:C:95:MET:HB2	2.49	0.43
1:B:214:GLU:O	1:B:227:PRO:HD3	2.18	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: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:72:GLY:O	1:C:73:SER:HB3	2.19	0.43
1:C:12:SER:C	1:C:14:GLY:H	2.21	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:C:216:GLU:O	1:C:218:VAL:HG23	2.19	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: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:C:54:ARG:HB2	1:C:54:ARG:HE	1.63	0.42
1:B:124:ARG:HH22	1:B:182:LYS:CG	2.32	0.42
1:B:48:ASP:OD2	1:B:50:ASP:HB2	2.19	0.42
1:C:145:ASN:N	1:C:145:ASN:ND2	2.66	0.42
1:C:51:VAL:O	1:C:54:ARG:HG2	2.19	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:B:8:ARG:HG3	1:B:12:SER:OG	2.20	0.42
1:A:201:ARG:NE	4:A:939:HOH:O	2.48	0.42
1:C:166:THR:HG23	1:C:167:GLN:N	2.34	0.42
1:B:26:LEU:HG	1:B:147:ASP:HB3	2.02	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:HD23	1:C:143:LEU:N	2.35	0.41
1:A:198:ARG:CD	1:A:221:HIS:O	2.68	0.41
1:C:11:GLY:O	1:C:13:ALA:N	2.53	0.41
1:B:152:GLN:HB3	1:B:152:GLN:HE21	1.53	0.41
1:A:146:HIS:HB2	1:A:157:HIS:NE2	2.35	0.41
1:C:80:TYR:CG	1:C:186:ILE:HD13	2.56	0.41
1:C:204:LEU:HD13	1:C:204:LEU:C	2.40	0.41
1:C:96:LEU:HD13	1:C:281:LEU:CD1	2.50	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:C:164:ASN:HD21	1:C:174:THR:CG2	2.33	0.41
1:B:124:ARG:HH22	1:B:182:LYS:CB	2.33	0.41
1:C:139:LEU:HD12	1:C:141:MET:HE1	2.03	0.41
1:C:122:SER:HB3	1:C:135:LEU:HA	2.02	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:268:VAL:CG1	1:C:269:ASP:N	2.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ILE:HG22	1:C:276:GLU:OE1	2.22	0.40
1:C:106:HIS:HA	1:C:204:LEU:HD23	2.04	0.40
1:C:7:VAL:HG23	1:C:79:GLY:C	2.42	0.40
1:A:121:ALA:CB	1:A:136:THR:HG22	2.51	0.40
1:C:148:THR:HA	1:C:153:GLU:O	2.21	0.40
1:B:93:MET:CE	1:B:288:ILE:HG12	2.52	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:118:GLU:HA	1:C:139:LEU:HD12	2.03	0.40
1:C:99:ASP:OD1	1:C:101:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/330 (82%)	256 (94%)	13 (5%)	3 (1%)	17	36
1	B	272/330 (82%)	251 (92%)	16 (6%)	5 (2%)	11	21
1	C	272/330 (82%)	217 (80%)	39 (14%)	16 (6%)	2	2
All	All	816/990 (82%)	724 (89%)	68 (8%)	24 (3%)	6	9

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 ⓘ

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%)	14	26
1	B	225/267 (84%)	213 (95%)	12 (5%)	28	53
1	C	225/267 (84%)	213 (95%)	12 (5%)	28	53
All	All	675/801 (84%)	632 (94%)	43 (6%)	22	43

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [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	A	600	-	3,3,3	0.63	0	2,2,2	0.17	0
3	EDO	A	601	-	3,3,3	0.64	0	2,2,2	0.31	0
3	EDO	A	606	-	3,3,3	0.70	0	2,2,2	0.25	0
3	EDO	A	608	-	3,3,3	0.65	0	2,2,2	0.28	0
3	EDO	A	612	-	3,3,3	0.68	0	2,2,2	0.17	0
3	EDO	B	602	-	3,3,3	0.68	0	2,2,2	0.26	0
3	EDO	B	604	-	3,3,3	0.63	0	2,2,2	0.29	0
3	EDO	B	605	-	3,3,3	0.64	0	2,2,2	0.25	0
3	EDO	B	607	-	3,3,3	0.63	0	2,2,2	0.30	0
3	EDO	B	610	-	3,3,3	0.64	0	2,2,2	0.31	0
3	EDO	C	603	-	3,3,3	0.65	0	2,2,2	0.21	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	A	600	-	-	0/1/1/1	0/0/0/0
3	EDO	A	601	-	-	0/1/1/1	0/0/0/0
3	EDO	A	606	-	-	0/1/1/1	0/0/0/0
3	EDO	A	608	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	612	-	-	0/1/1/1	0/0/0/0
3	EDO	B	602	-	-	0/1/1/1	0/0/0/0
3	EDO	B	604	-	-	0/1/1/1	0/0/0/0
3	EDO	B	605	-	-	0/1/1/1	0/0/0/0
3	EDO	B	607	-	-	0/1/1/1	0/0/0/0
3	EDO	B	610	-	-	0/1/1/1	0/0/0/0
3	EDO	C	603	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	EDO	1	0
3	A	612	EDO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/330 (83%)	0.06	16 (5%) 26 20	26, 45, 73, 104	0
1	B	276/330 (83%)	0.16	16 (5%) 26 20	29, 49, 84, 116	0
1	C	276/330 (83%)	1.62	83 (30%) 1 0	56, 105, 152, 161	0
All	All	827/990 (83%)	0.61	115 (13%) 4 2	26, 59, 139, 161	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	GLY	9.7
1	C	268	VAL	9.6
1	C	134	VAL	9.3
1	C	307	GLY	8.4
1	B	306	PRO	7.8
1	C	127	THR	7.1
1	C	267	HIS	6.9
1	C	24	TYR	6.8
1	C	22	ASN	6.6
1	C	71	ASP	6.4
1	C	73	SER	6.4
1	A	307	GLY	6.2
1	B	180	VAL	6.2
1	C	126	MET	6.1
1	C	129	GLY	6.1
1	C	306	PRO	6.1
1	C	75	ARG	5.9
1	C	70	GLN	5.9
1	C	272	ILE	5.9
1	C	74	ASN	5.7
1	C	72	GLY	5.6
1	C	23	TYR	5.5
1	A	306	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	69	MET	5.3
1	C	128	ASP	5.2
1	C	29	MET	5.1
1	C	125	VAL	5.1
1	C	150	ARG	5.1
1	C	269	ASP	4.7
1	C	20	LYS	4.6
1	C	161	VAL	4.6
1	C	63	GLY	4.5
1	C	66	LEU	4.4
1	C	172	TRP	4.4
1	C	15	ASN	4.4
1	C	131	SER	4.3
1	C	28	SER	4.3
1	C	167	GLN	4.3
1	C	21	ASP	4.3
1	C	130	GLN	4.2
1	C	163	ALA	4.2
1	C	271	GLU	4.2
1	C	42	GLY	4.1
1	C	166	THR	4.1
1	C	141	MET	4.1
1	C	151	ASP	4.1
1	B	72	GLY	4.1
1	C	132	GLU	4.0
1	C	162	VAL	3.9
1	B	182	LYS	3.9
1	C	152	GLN	3.8
1	C	140	VAL	3.7
1	B	181	GLY	3.7
1	C	282	LYS	3.7
1	C	182	LYS	3.5
1	B	75	ARG	3.5
1	C	39	GLU	3.4
1	A	182	LYS	3.3
1	C	235	SER	3.3
1	C	16	TYR	3.3
1	C	8	ARG	3.3
1	B	163	ALA	3.3
1	C	173	LYS	3.2
1	C	65	ASP	3.1
1	B	162	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	69	MET	3.1
1	C	76	HIS	3.0
1	A	72	GLY	3.0
1	C	60	LEU	3.0
1	C	142	ALA	3.0
1	C	91	SER	3.0
1	C	305	THR	2.9
1	C	293	ASP	2.9
1	C	283	GLU	2.9
1	C	41	LEU	2.9
1	B	70	GLN	2.8
1	C	160	ALA	2.8
1	C	291	TYR	2.8
1	C	80	TYR	2.7
1	C	294	ALA	2.7
1	C	270	PRO	2.6
1	C	233	ALA	2.6
1	A	161	VAL	2.6
1	C	17	TYR	2.5
1	A	162	VAL	2.5
1	C	43	LEU	2.5
1	A	163	ALA	2.5
1	B	130	GLN	2.4
1	C	139	LEU	2.4
1	C	90	VAL	2.4
1	B	71	ASP	2.3
1	C	27	GLY	2.3
1	B	183	THR	2.3
1	C	68	ARG	2.3
1	C	79	GLY	2.3
1	A	130	GLN	2.3
1	B	141	MET	2.3
1	A	94	ALA	2.3
1	C	276	GLU	2.3
1	A	8	ARG	2.3
1	A	90	VAL	2.3
1	A	70	GLN	2.2
1	C	164	ASN	2.2
1	B	140	VAL	2.2
1	C	19	ASP	2.2
1	A	91	SER	2.2
1	C	38	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	153	GLU	2.1
1	A	279	GLN	2.1
1	C	286	PHE	2.1
1	A	28	SER	2.1
1	C	13	ALA	2.0
1	B	1	MET	2.0
1	C	168	HIS	2.0
1	C	82	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	B	605	4/4	0.92	0.41	8.07	68,69,70,70	0
3	EDO	A	612	4/4	0.89	0.42	6.71	57,59,59,61	0
3	EDO	A	600	4/4	0.92	0.31	5.01	63,64,65,65	0
3	EDO	B	610	4/4	0.91	0.35	3.77	84,84,85,85	0
3	EDO	C	603	4/4	0.83	0.38	3.76	89,89,89,90	0
3	EDO	A	601	4/4	0.94	0.20	-	84,85,86,87	0
2	MG	A	900	1/1	0.99	0.10	-	36,36,36,36	0
3	EDO	A	608	4/4	0.78	0.17	-	75,78,78,78	0
3	EDO	B	602	4/4	0.76	0.20	-	74,76,77,79	0
3	EDO	B	604	4/4	0.93	0.48	-	86,86,86,86	0
3	EDO	A	606	4/4	0.87	0.24	-	76,78,78,79	0
2	MG	C	902	1/1	0.95	0.32	-	78,78,78,78	0
3	EDO	B	607	4/4	0.56	0.39	-	114,114,114,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	B	901	1/1	0.94	0.28	-	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.