Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2026 – 11:23 AM EDT

PDB ID	:	37RI / pdb_000037ri
Title	:	Multi-parameter optimization of a novel anti-TROP2 MMAE Antibody-Drug -Conjugate for solid tumor therapy
Authors	:	Chrencik, J.E.
Deposited on	:	2026-08-01
Resolution	:	2.30 Å(reported)

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

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

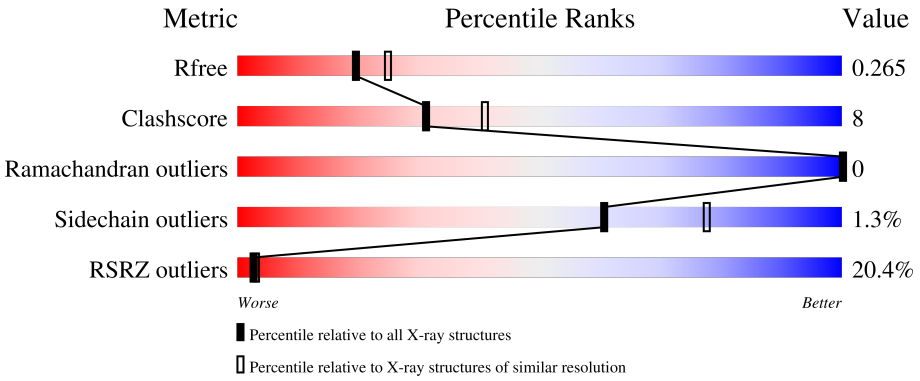
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



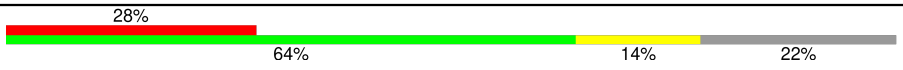
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	241	8% 73% 17% 10%
1	C	241	11% 78% 12% 10%
2	B	234	79% 13% 9%
2	D	234	% 82% 9% 9%
3	E	284	49% 57% 23% 20%

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Mol	Chain	Length	Quality of chain
3	F	284	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10476 atoms, of which 12 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 MK6837 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1645	1051	267	321	6			
1	C	217	Total	C	N	O	S	0	0	0
			1636	1045	265	320	6			

- Molecule 2 is a protein called MK6837 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1640	1029	273	333	5			
2	D	213	Total	C	N	O	S	0	1	0
			1643	1031	273	335	4			

- Molecule 3 is a protein called Tumor-associated calcium signal transducer 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	227	Total	C	N	O	S	0	0	0
			1751	1084	324	328	15			
3	F	222	Total	C	N	O	S	0	0	0
			1723	1064	324	320	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	MET	-	expression tag	UNP P09758
E	-8	ALA	-	expression tag	UNP P09758
E	-7	MET	-	expression tag	UNP P09758
E	-6	LYS	-	expression tag	UNP P09758
E	-5	PHE	-	expression tag	UNP P09758
E	-4	LEU	-	expression tag	UNP P09758
E	-3	VAL	-	expression tag	UNP P09758
E	-2	ASN	-	expression tag	UNP P09758

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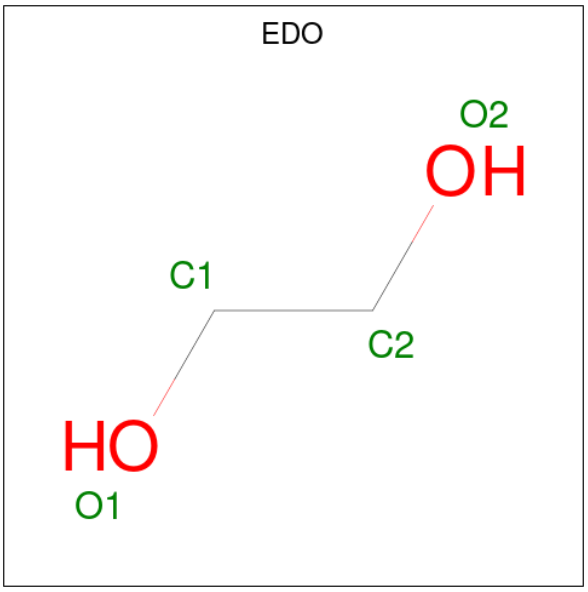
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	VAL	-	expression tag	UNP P09758
E	0	ALA	-	expression tag	UNP P09758
E	1	LEU	-	expression tag	UNP P09758
E	2	VAL	-	expression tag	UNP P09758
E	3	PHE	-	expression tag	UNP P09758
E	4	MET	-	expression tag	UNP P09758
E	5	VAL	-	expression tag	UNP P09758
E	6	VAL	-	expression tag	UNP P09758
E	7	TYR	-	expression tag	UNP P09758
E	8	ILE	-	expression tag	UNP P09758
E	9	SER	-	expression tag	UNP P09758
E	10	TYR	-	expression tag	UNP P09758
E	11	ILE	-	expression tag	UNP P09758
E	12	TYR	-	expression tag	UNP P09758
E	13	ALA	-	expression tag	UNP P09758
E	14	HIS	-	expression tag	UNP P09758
E	15	HIS	-	expression tag	UNP P09758
E	16	HIS	-	expression tag	UNP P09758
E	17	HIS	-	expression tag	UNP P09758
E	18	HIS	-	expression tag	UNP P09758
E	19	HIS	-	expression tag	UNP P09758
E	20	HIS	-	expression tag	UNP P09758
E	21	HIS	-	expression tag	UNP P09758
E	22	HIS	-	expression tag	UNP P09758
E	23	HIS	-	expression tag	UNP P09758
E	24	GLU	-	expression tag	UNP P09758
E	25	ASN	-	expression tag	UNP P09758
E	26	LEU	-	expression tag	UNP P09758
E	27	TYR	-	expression tag	UNP P09758
E	28	PHE	-	expression tag	UNP P09758
E	29	GLN	-	expression tag	UNP P09758
E	30	GLY	-	expression tag	UNP P09758
F	-9	MET	-	expression tag	UNP P09758
F	-8	ALA	-	expression tag	UNP P09758
F	-7	MET	-	expression tag	UNP P09758
F	-6	LYS	-	expression tag	UNP P09758
F	-5	PHE	-	expression tag	UNP P09758
F	-4	LEU	-	expression tag	UNP P09758
F	-3	VAL	-	expression tag	UNP P09758
F	-2	ASN	-	expression tag	UNP P09758
F	-1	VAL	-	expression tag	UNP P09758
F	0	ALA	-	expression tag	UNP P09758

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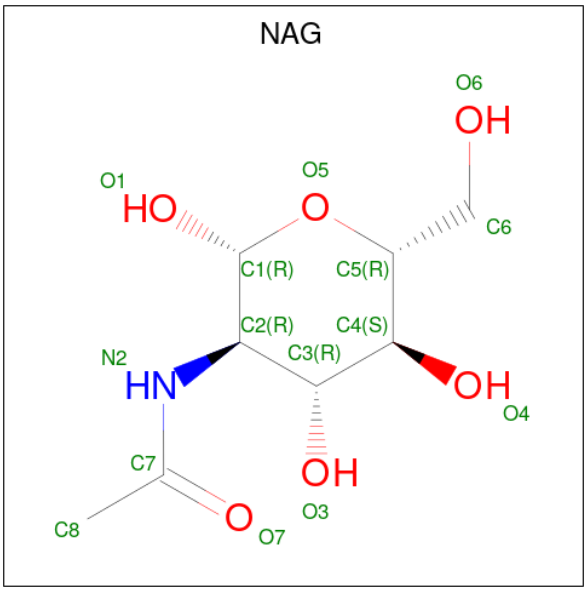
Chain	Residue	Modelled	Actual	Comment	Reference
F	1	LEU	-	expression tag	UNP P09758
F	2	VAL	-	expression tag	UNP P09758
F	3	PHE	-	expression tag	UNP P09758
F	4	MET	-	expression tag	UNP P09758
F	5	VAL	-	expression tag	UNP P09758
F	6	VAL	-	expression tag	UNP P09758
F	7	TYR	-	expression tag	UNP P09758
F	8	ILE	-	expression tag	UNP P09758
F	9	SER	-	expression tag	UNP P09758
F	10	TYR	-	expression tag	UNP P09758
F	11	ILE	-	expression tag	UNP P09758
F	12	TYR	-	expression tag	UNP P09758
F	13	ALA	-	expression tag	UNP P09758
F	14	HIS	-	expression tag	UNP P09758
F	15	HIS	-	expression tag	UNP P09758
F	16	HIS	-	expression tag	UNP P09758
F	17	HIS	-	expression tag	UNP P09758
F	18	HIS	-	expression tag	UNP P09758
F	19	HIS	-	expression tag	UNP P09758
F	20	HIS	-	expression tag	UNP P09758
F	21	HIS	-	expression tag	UNP P09758
F	22	HIS	-	expression tag	UNP P09758
F	23	HIS	-	expression tag	UNP P09758
F	24	GLU	-	expression tag	UNP P09758
F	25	ASN	-	expression tag	UNP P09758
F	26	LEU	-	expression tag	UNP P09758
F	27	TYR	-	expression tag	UNP P09758
F	28	PHE	-	expression tag	UNP P09758
F	29	GLN	-	expression tag	UNP P09758
F	30	GLY	-	expression tag	UNP P09758

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

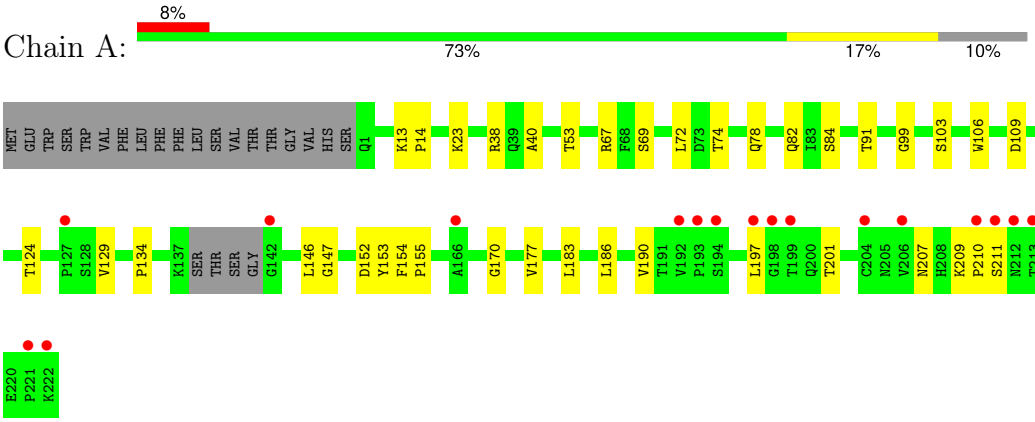
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	73	Total O 73 73	0	0
6	B	92	Total O 92 92	0	0
6	C	77	Total O 77 77	0	0
6	D	92	Total O 92 92	0	0
6	E	22	Total O 22 22	0	0
6	F	26	Total O 26 26	0	0

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.

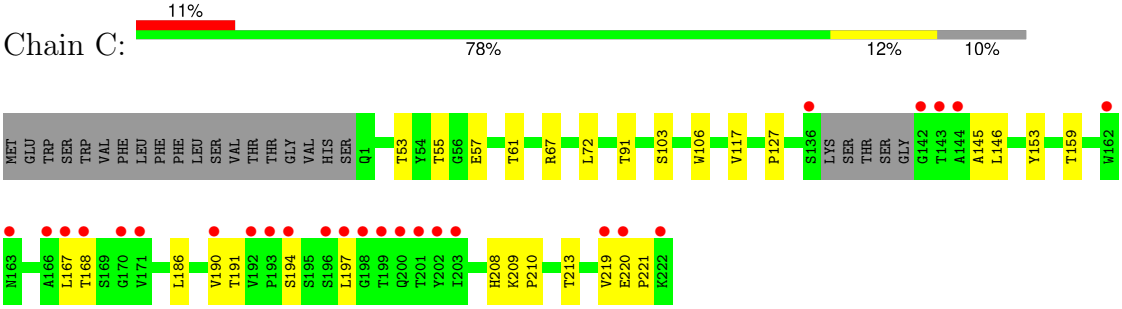
• Molecule 1: MK6837 Heavy Chain

Chain A:



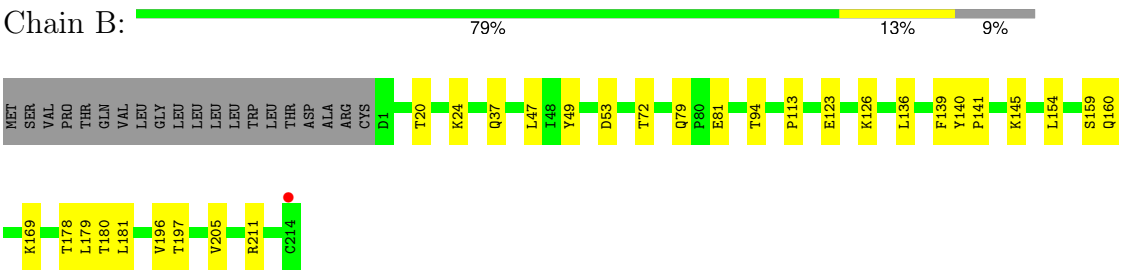
• Molecule 1: MK6837 Heavy Chain

Chain C:



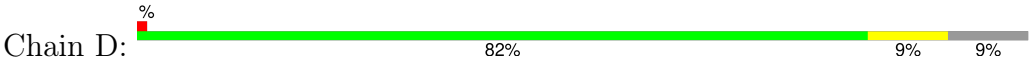
• Molecule 2: MK6837 Light Chain

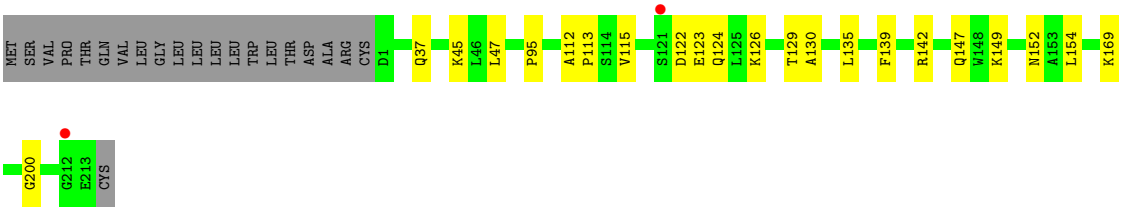
Chain B:



• Molecule 2: MK6837 Light Chain

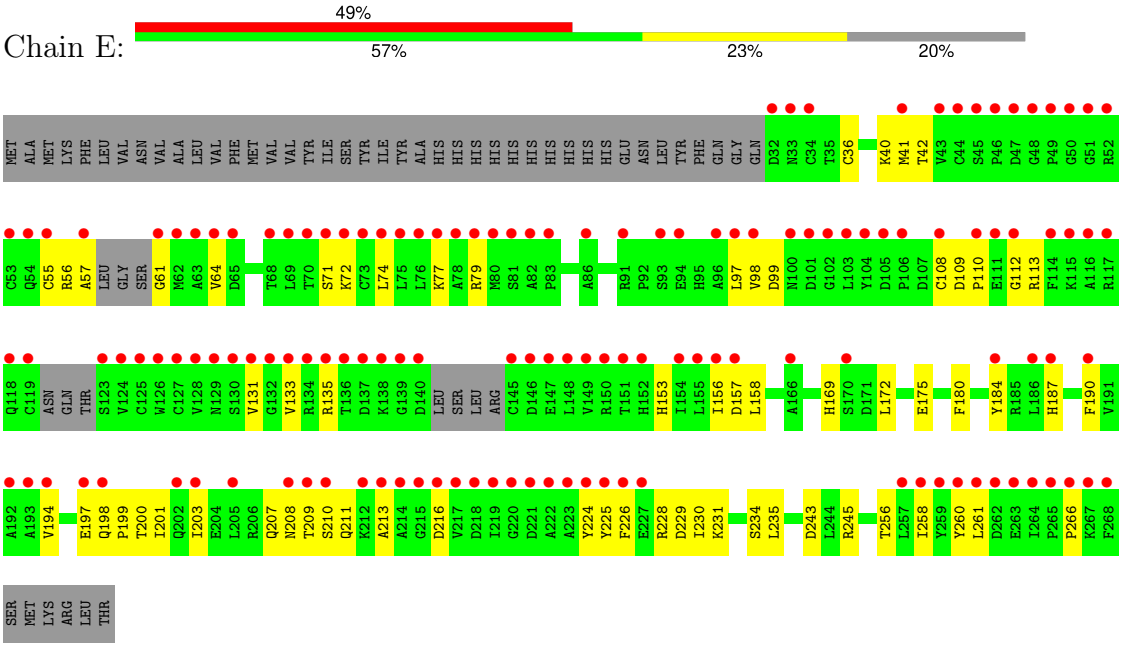
Chain D:





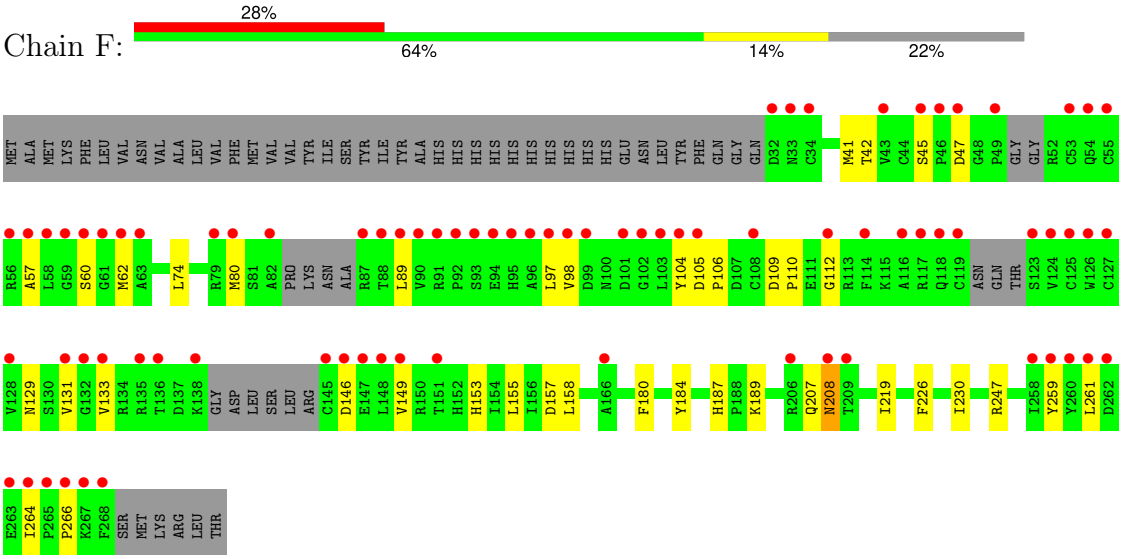
• Molecule 3: Tumor-associated calcium signal transducer 2

Chain E:



• Molecule 3: Tumor-associated calcium signal transducer 2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.78Å 212.07Å 77.44Å 90.00° 106.02° 90.00°	Depositor
Resolution (Å)	37.22 – 2.30 37.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (37.22-2.30) 95.6 (37.22-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.29Å)	Xtriage
Refinement program	PHENIX (2.2_6143: ???)	Depositor
R, R_{free}	0.227 , 0.265 0.227 , 0.265	Depositor DCC
R_{free} test set	3239 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10476	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: EDO, NAG

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	0.29	0/1690	0.50	0/2304
1	C	0.30	0/1681	0.53	0/2293
2	B	0.29	0/1676	0.50	0/2279
2	D	0.28	0/1679	0.48	0/2283
3	E	0.23	0/1783	0.46	0/2409
3	F	0.26	0/1752	0.51	0/2365
All	All	0.28	0/10261	0.50	0/13933

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	1645	0	1588	25	0
1	C	1636	0	1575	16	0
2	B	1640	0	1601	18	0
2	D	1643	0	1601	15	0
3	E	1751	0	1669	61	0
3	F	1723	0	1654	32	0
4	A	4	6	6	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	6	0	0
4	C	4	6	6	0	0
4	D	4	0	6	0	0
5	E	14	0	13	0	0
5	F	14	0	13	2	0
6	A	73	0	0	3	0
6	B	92	0	0	0	0
6	C	77	0	0	0	0
6	D	92	0	0	2	0
6	E	22	0	0	0	0
6	F	26	0	0	0	0
All	All	10464	12	9738	163	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 8.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:GLN:HG2	2:D:129:THR:O	1.70	0.90
3:E:156:ILE:HB	3:E:203:ILE:HG22	1.56	0.88
3:F:62:MET:HE1	3:F:110:PRO:O	1.78	0.84
3:E:156:ILE:HD13	3:E:258:ILE:HG12	1.59	0.83
3:F:41:MET:HA	3:F:41:MET:HE2	1.62	0.81
3:F:247:ARG:HH22	5:F:301:NAG:H62	1.44	0.81
3:E:156:ILE:HB	3:E:203:ILE:CG2	2.11	0.80
3:E:172:LEU:HD21	3:E:201:ILE:HG23	1.65	0.79
3:E:197:GLU:HB2	3:F:89:LEU:HD11	1.67	0.77
3:E:74:LEU:HD21	3:E:112:GLY:HA2	1.67	0.76
3:F:80:MET:HE1	3:F:105:ASP:N	2.02	0.75
3:E:40:LYS:HE2	3:E:234:SER:O	1.86	0.75
3:E:42:THR:HG22	3:E:57:ALA:HA	1.70	0.72
1:A:129:VAL:HG23	6:A:412:HOH:O	1.90	0.71
3:F:153:HIS:HB3	3:F:261:LEU:HB3	1.73	0.71
2:D:113:PRO:HB3	2:D:139:PHE:HB3	1.72	0.71
3:E:228:ARG:HG2	3:E:235:LEU:HD21	1.73	0.70
3:E:226:PHE:O	3:E:230:ILE:HG12	1.91	0.70
3:F:247:ARG:NH2	5:F:301:NAG:H62	2.05	0.69
3:F:129:ASN:OD1	3:F:133:VAL:HG22	1.95	0.66
3:E:157:ASP:O	3:E:158:LEU:HD23	1.96	0.65
3:E:77:LYS:HD3	3:E:108:CYS:SG	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:THR:HG22	1:A:211:SER:HB3	1.80	0.64
3:E:226:PHE:CE1	3:E:230:ILE:HD11	2.33	0.64
1:C:55:THR:OG1	1:C:57:GLU:HG3	1.99	0.62
3:E:172:LEU:HD21	3:E:201:ILE:CG2	2.30	0.62
3:E:228:ARG:NH1	3:E:231:LYS:HE2	2.15	0.62
1:C:208:HIS:HB3	1:C:213:THR:OG1	2.00	0.62
3:E:97:LEU:HD11	3:F:266:PRO:HG2	1.82	0.62
3:E:109:ASP:HB2	3:E:110:PRO:HD2	1.81	0.62
2:D:122:ASP:O	2:D:126:LYS:HG3	2.00	0.61
3:E:213:ALA:HB3	3:E:216:ASP:OD2	2.01	0.60
3:F:109:ASP:HB2	3:F:110:PRO:HD2	1.83	0.60
3:E:180:PHE:HA	3:E:184:TYR:HD2	1.67	0.59
3:E:187:HIS:HB3	3:E:190:PHE:CE2	2.39	0.57
3:E:135:ARG:NH2	3:E:266:PRO:HA	2.20	0.57
3:F:62:MET:HE1	3:F:110:PRO:C	2.30	0.57
1:A:23:LYS:HG3	1:A:78:GLN:HG2	1.87	0.56
3:E:156:ILE:HD13	3:E:258:ILE:HG23	1.86	0.56
2:B:211:ARG:HH11	2:B:211:ARG:HG2	1.71	0.56
3:E:194:VAL:HG22	3:E:203:ILE:CD1	2.36	0.56
1:C:127:PRO:HB3	1:C:153:TYR:HB3	1.87	0.56
1:C:167:LEU:HD21	1:C:190:VAL:HG21	1.88	0.56
3:F:42:THR:HG22	3:F:57:ALA:HA	1.88	0.55
1:A:207:ASN:OD1	1:A:209:LYS:HD2	2.05	0.55
3:E:190:PHE:CE1	3:E:207:GLN:HG3	2.41	0.55
3:F:74:LEU:HD21	3:F:112:GLY:HA2	1.88	0.55
1:A:53:THR:HA	1:A:72:LEU:HD11	1.89	0.55
1:A:13:LYS:HD3	1:A:121:SER:HA	1.89	0.53
3:E:56:ARG:HH21	3:E:61:GLY:HA3	1.74	0.53
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.91	0.53
3:E:157:ASP:C	3:E:158:LEU:HD23	2.33	0.53
2:B:20:THR:HG23	2:B:72:THR:HG23	1.91	0.53
3:E:72:LYS:HD2	3:E:224:TYR:HB2	1.91	0.53
3:E:158:LEU:CD1	3:E:230:ILE:HD12	2.39	0.53
2:D:142:ARG:HG2	6:D:477:HOH:O	2.08	0.53
3:E:194:VAL:HG22	3:E:203:ILE:HD13	1.91	0.53
1:A:154:PHE:HB2	1:A:183:LEU:HD13	1.90	0.52
1:C:194:SER:O	1:C:197:LEU:HG	2.09	0.52
3:E:213:ALA:HB3	3:E:216:ASP:CG	2.34	0.52
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.91	0.52
3:E:40:LYS:CE	3:E:234:SER:O	2.58	0.52
3:E:156:ILE:CD1	3:E:258:ILE:HG12	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:131:VAL:HG21	3:E:260:TYR:CD2	2.45	0.52
2:D:112:ALA:HB2	2:D:200:GLY:O	2.09	0.52
2:D:113:PRO:CB	2:D:139:PHE:HB3	2.40	0.52
3:E:74:LEU:HA	3:E:77:LYS:HG3	1.92	0.52
1:C:219:VAL:O	1:C:219:VAL:HG23	2.10	0.52
1:A:134:PRO:HG3	1:A:197:LEU:HD22	1.92	0.51
3:E:109:ASP:OD2	3:E:113:ARG:HB2	2.11	0.51
3:E:55:CYS:O	3:E:64:VAL:HG12	2.11	0.51
3:E:229:ASP:OD1	3:E:234:SER:HA	2.11	0.51
3:E:169:HIS:NE2	3:E:194:VAL:O	2.35	0.50
3:E:266:PRO:HG3	3:F:97:LEU:HD21	1.92	0.50
1:C:186:LEU:HD12	1:C:186:LEU:C	2.36	0.50
3:F:131:VAL:HG23	3:F:133:VAL:HG13	1.93	0.50
3:E:131:VAL:HG23	3:E:133:VAL:HG23	1.94	0.50
3:E:187:HIS:HB3	3:E:190:PHE:CD2	2.47	0.50
1:C:145:ALA:HB2	1:C:191:THR:HG22	1.93	0.50
1:A:67:ARG:HB3	1:A:84:SER:O	2.10	0.50
3:E:41:MET:HE2	3:E:79:ARG:HG2	1.94	0.49
1:A:103:SER:HA	1:A:106:TRP:CE3	2.48	0.49
2:B:20:THR:HG23	2:B:72:THR:CG2	2.43	0.49
3:E:98:VAL:HG12	3:E:99:ASP:N	2.28	0.49
3:F:226:PHE:CE2	3:F:230:ILE:HD11	2.47	0.49
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.95	0.49
3:E:190:PHE:CD1	3:E:207:GLN:HG3	2.48	0.49
3:F:57:ALA:HB3	3:F:60:SER:O	2.12	0.49
3:E:226:PHE:CZ	3:E:230:ILE:HD11	2.48	0.48
1:A:177:VAL:HG23	6:A:445:HOH:O	2.13	0.48
1:A:155:PRO:HD2	1:A:210:PRO:CB	2.44	0.48
1:A:146:LEU:HD12	1:A:147:GLY:N	2.29	0.48
1:C:146:LEU:HD12	1:C:219:VAL:HG23	1.96	0.47
2:B:179:LEU:HG	2:B:181:LEU:HD21	1.96	0.47
2:D:123:GLU:OE1	2:D:123:GLU:N	2.36	0.47
2:B:79:GLN:HB3	2:B:81:GLU:OE1	2.15	0.47
3:F:45:SER:HB2	3:F:47:ASP:OD2	2.14	0.47
2:B:211:ARG:HG2	2:B:211:ARG:NH1	2.29	0.47
3:F:149:VAL:CG2	3:F:264:ILE:HD11	2.45	0.47
3:E:169:HIS:HE2	3:E:194:VAL:C	2.23	0.47
1:C:61:THR:HG22	2:D:95:PRO:HB3	1.97	0.46
3:E:228:ARG:CG	3:E:235:LEU:HD21	2.44	0.46
2:B:136:LEU:HD21	2:B:196:VAL:HG13	1.96	0.46
2:B:179:LEU:HG	2:B:181:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:HB2	1:A:183:LEU:CD1	2.46	0.46
2:D:147:GLN:CD	2:D:154:LEU:HD11	2.41	0.46
2:B:49:TYR:O	2:B:53:ASP:HB2	2.16	0.46
1:C:91:THR:HA	1:C:117:VAL:O	2.15	0.46
3:E:208:ASN:OD1	3:E:211:GLN:HG3	2.16	0.46
3:E:198:GLN:HA	3:E:199:PRO:HA	1.76	0.45
3:E:235:LEU:HD22	3:E:235:LEU:N	2.30	0.45
1:C:146:LEU:CD1	1:C:219:VAL:HG23	2.47	0.45
1:A:38:ARG:HH12	1:A:40:ALA:HB2	1.81	0.45
1:A:186:LEU:C	1:A:186:LEU:HD12	2.43	0.44
2:D:115:VAL:HA	2:D:135:LEU:O	2.16	0.44
3:F:146:ASP:OD1	3:F:146:ASP:N	2.49	0.44
3:F:149:VAL:HG21	3:F:264:ILE:HD11	1.97	0.44
3:E:175:GLU:HG2	3:E:245:ARG:O	2.17	0.44
1:C:53:THR:HA	1:C:72:LEU:HD11	1.99	0.44
3:E:36:CYS:HB2	3:E:55:CYS:SG	2.56	0.44
3:F:180:PHE:HA	3:F:184:TYR:HD2	1.82	0.44
1:A:153:TYR:C	1:A:183:LEU:HD12	2.43	0.44
1:C:209:LYS:N	1:C:210:PRO:CD	2.81	0.43
1:C:220:GLU:HB2	1:C:221:PRO:HD2	2.00	0.43
3:E:197:GLU:O	3:E:198:GLN:C	2.61	0.43
3:F:264:ILE:HG13	3:F:264:ILE:O	2.19	0.43
3:E:225:TYR:CE1	3:E:235:LEU:HB2	2.53	0.43
1:A:69:SER:OG	1:A:82:GLN:HB3	2.19	0.43
2:B:145:LYS:HB3	2:B:197:THR:HB	2.01	0.43
3:F:207:GLN:HB2	3:F:219:ILE:CG2	2.48	0.43
1:A:14:PRO:HD3	1:A:120:SER:C	2.44	0.43
3:F:187:HIS:ND1	3:F:189:LYS:HG2	2.33	0.43
1:A:99:GLY:HA2	4:A:301:EDO:H21	2.00	0.43
3:E:135:ARG:CZ	3:E:266:PRO:HA	2.49	0.42
4:A:301:EDO:H12	6:A:440:HOH:O	2.17	0.42
3:E:228:ARG:HB3	3:E:235:LEU:CD2	2.49	0.42
3:F:157:ASP:O	3:F:158:LEU:HD23	2.19	0.42
2:B:159:SER:HA	2:B:178:THR:O	2.20	0.42
2:D:169:LYS:HD3	2:D:169:LYS:HA	1.79	0.42
1:A:152:ASP:HA	1:A:183:LEU:HB3	2.01	0.42
2:B:140:TYR:CG	2:B:141:PRO:HA	2.55	0.41
3:E:42:THR:HG21	3:E:64:VAL:HG11	2.01	0.41
3:E:158:LEU:CD2	3:E:256:THR:HG23	2.50	0.41
3:E:243:ASP:O	3:E:245:ARG:HG3	2.20	0.41
1:A:177:VAL:HG11	2:B:160:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:LYS:HD2	6:D:431:HOH:O	2.19	0.41
1:A:170:GLY:O	1:A:190:VAL:HA	2.20	0.41
2:D:149:LYS:HD3	2:D:152:ASN:HA	2.02	0.41
2:B:180:THR:C	2:B:181:LEU:HD22	2.46	0.41
3:F:104:TYR:O	3:F:106:PRO:HD3	2.19	0.41
1:C:103:SER:HA	1:C:106:TRP:CE3	2.56	0.41
2:D:129:THR:HG22	2:D:130:ALA:N	2.36	0.41
2:B:169:LYS:HD3	2:B:169:LYS:HA	1.96	0.41
1:A:109:ASP:OD1	4:A:301:EDO:H22	2.21	0.41
2:B:123:GLU:HA	2:B:126:LYS:HD2	2.02	0.41
3:E:208:ASN:OD1	3:E:210:SER:HB3	2.21	0.41
3:F:155:LEU:HD23	3:F:259:TYR:HD2	1.86	0.41
1:A:91:THR:HA	1:A:117:VAL:O	2.20	0.40
3:E:153:HIS:HB3	3:E:261:LEU:HB3	2.04	0.40
3:F:187:HIS:CE1	3:F:189:LYS:HD2	2.56	0.40
3:F:155:LEU:HD23	3:F:259:TYR:CD2	2.57	0.40
3:F:157:ASP:C	3:F:158:LEU:HD23	2.46	0.40
3:F:208:ASN:OD1	3:F:208:ASN:N	2.54	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	214/241 (89%)	209 (98%)	5 (2%)	0	100	100
1	C	213/241 (88%)	207 (97%)	6 (3%)	0	100	100
2	B	212/234 (91%)	206 (97%)	6 (3%)	0	100	100
2	D	212/234 (91%)	204 (96%)	8 (4%)	0	100	100
3	E	219/284 (77%)	208 (95%)	11 (5%)	0	100	100
3	F	212/284 (75%)	206 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1282/1518 (84%)	1240 (97%)	42 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	182/205 (89%)	180 (99%)	2 (1%)	65 81
1	C	181/205 (88%)	178 (98%)	3 (2%)	53 72
2	B	188/206 (91%)	184 (98%)	4 (2%)	47 66
2	D	188/206 (91%)	188 (100%)	0	100 100
3	E	184/247 (74%)	181 (98%)	3 (2%)	55 73
3	F	183/247 (74%)	181 (99%)	2 (1%)	65 81
All	All	1106/1316 (84%)	1092 (99%)	14 (1%)	61 77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	201	THR
2	B	24	LYS
2	B	94	THR
2	B	154	LEU
2	B	205	VAL
1	C	67	ARG
1	C	159	THR
1	C	168	THR
3	E	71	SER
3	E	200	THR
3	E	209	THR
3	F	98	VAL
3	F	208	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	37	GLN
2	B	147	GLN
2	B	160	GLN
1	C	212	ASN
2	D	3	GLN
2	D	79	GLN
2	D	147	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
4	EDO	D	301	-	3,3,3	0.24	0	2,2,2	0.33	0
5	NAG	E	301	3	14,14,15	0.66	0	17,19,21	0.91	1 (5%)
4	EDO	B	301	-	3,3,3	0.25	0	2,2,2	0.39	0
5	NAG	F	301	3	14,14,15	0.71	0	17,19,21	0.92	0
4	EDO	C	301	-	3,3,3	0.21	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	A	301	-	3,3,3	0.29	0	2,2,2	0.45	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
4	EDO	D	301	-	-	1/1/1/1	-
5	NAG	E	301	3	-	0/6/23/26	0/1/1/1
4	EDO	B	301	-	-	0/1/1/1	-
5	NAG	F	301	3	-	0/6/23/26	0/1/1/1
4	EDO	C	301	-	-	0/1/1/1	-
4	EDO	A	301	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	301	NAG	C1-O5-C5	2.37	115.37	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	301	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	301	NAG	2	0
4	A	301	EDO	3	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, 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	218/241 (90%)	0.54	20 (9%) 14 16	20, 43, 87, 98	0
1	C	217/241 (90%)	0.43	26 (11%) 9 9	19, 40, 92, 112	0
2	B	214/234 (91%)	0.06	1 (0%) 87 87	22, 38, 64, 95	0
2	D	213/234 (91%)	0.06	2 (0%) 81 82	22, 39, 65, 85	1 (0%)
3	E	227/284 (79%)	2.43	138 (60%) 0 0	31, 82, 146, 170	0
3	F	222/284 (78%)	1.63	80 (36%) 1 1	27, 71, 128, 146	0
All	All	1311/1518 (86%)	0.88	267 (20%) 3 3	19, 47, 116, 170	1 (0%)

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	140	ASP	6.8
3	E	149	VAL	6.4
3	E	128	VAL	6.4
3	F	88	THR	6.1
3	E	148	LEU	5.9
3	E	125	CYS	5.9
3	E	116	ALA	5.9
3	F	57	ALA	5.8
3	E	123	SER	5.8
3	E	57	ALA	5.7
3	E	214	ALA	5.7
3	F	97	LEU	5.7
3	F	98	VAL	5.5
3	E	264	ILE	5.4
3	E	133	VAL	5.4
3	E	126	TRP	5.3
3	F	268	PHE	5.2
3	E	222	ALA	5.2
3	E	75	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
3	E	260	TYR	4.9
3	E	268	PHE	4.9
3	E	213	ALA	4.8
3	E	131	VAL	4.8
3	F	148	LEU	4.7
3	E	124	VAL	4.7
3	E	127	CYS	4.7
3	F	123	SER	4.6
3	E	219	ILE	4.5
3	E	78	ALA	4.5
3	F	264	ILE	4.4
3	E	154	ILE	4.4
3	E	119	CYS	4.3
3	E	71	SER	4.3
3	E	63	ALA	4.2
3	E	106	PRO	4.2
3	F	90	VAL	4.2
3	E	112	GLY	4.2
3	F	149	VAL	4.1
3	E	266	PRO	4.1
3	E	104	TYR	4.1
3	F	103	LEU	4.1
3	E	108	CYS	4.1
3	E	151	THR	4.1
3	F	124	VAL	4.1
3	E	209	THR	4.0
3	E	145	CYS	4.0
3	E	114	PHE	4.0
3	F	32	ASP	4.0
3	E	117	ARG	4.0
3	F	56	ARG	3.9
3	F	96	ALA	3.9
3	F	99	ASP	3.9
3	F	58	LEU	3.9
3	E	138	LYS	3.9
3	F	208	ASN	3.9
3	E	51	GLY	3.8
1	C	166	ALA	3.8
3	F	119	CYS	3.8
3	E	134	ARG	3.8
3	E	47	ASP	3.8
3	E	205	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
3	F	89	LEU	3.7
3	E	103	LEU	3.7
3	E	43	VAL	3.7
3	F	265	PRO	3.7
3	E	136	THR	3.7
3	E	190	PHE	3.6
3	F	93	SER	3.5
3	F	61	GLY	3.5
3	E	132	GLY	3.5
3	F	45	SER	3.5
3	F	147	GLU	3.5
3	F	126	TRP	3.5
3	E	258	ILE	3.5
3	F	117	ARG	3.4
3	E	54	GLN	3.4
3	E	129	ASN	3.4
3	E	227	GLU	3.4
3	E	34	CYS	3.4
3	F	43	VAL	3.4
3	E	110	PRO	3.3
3	F	46	PRO	3.3
3	E	82	ALA	3.3
3	E	155	LEU	3.3
3	F	261	LEU	3.3
3	E	64	VAL	3.3
3	F	116	ALA	3.3
3	F	146	ASP	3.3
3	F	60	SER	3.3
3	E	105	ASP	3.2
3	F	114	PHE	3.2
2	D	212	GLY	3.2
3	E	135	ARG	3.2
1	A	199	THR	3.2
1	C	196	SER	3.2
3	F	79	ARG	3.2
3	F	82	ALA	3.2
3	E	50	GLY	3.2
3	E	100	ASN	3.2
3	E	220	GLY	3.2
3	E	65	ASP	3.2
3	E	221	ASP	3.2
2	B	214	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
3	E	139	GLY	3.1
3	E	261	LEU	3.1
3	F	136	THR	3.1
3	E	44	CYS	3.1
1	A	197	LEU	3.1
1	C	162	TRP	3.1
3	F	262	ASP	3.1
3	E	166	ALA	3.1
3	E	223	ALA	3.1
3	F	128	VAL	3.1
3	E	74	LEU	3.1
3	E	186	LEU	3.1
3	F	92	PRO	3.1
3	E	259	TYR	3.1
3	F	151	THR	3.1
3	E	73	CYS	3.1
3	F	125	CYS	3.1
3	E	46	PRO	3.1
3	E	217	VAL	3.1
3	E	147	GLU	3.0
1	A	219	VAL	3.0
3	E	150	ARG	3.0
3	E	226	PHE	3.0
3	E	80	MET	3.0
3	F	145	CYS	3.0
3	F	131	VAL	3.0
3	E	69	LEU	2.9
3	F	94	GLU	2.9
3	E	212	LYS	2.9
3	E	118	GLN	2.9
1	A	212	ASN	2.9
3	E	33	ASN	2.9
3	E	218	ASP	2.9
3	E	197	GLU	2.9
3	E	263	GLU	2.9
3	E	61	GLY	2.9
3	E	215	GLY	2.9
1	A	210	PRO	2.9
1	C	197	LEU	2.9
1	C	168	THR	2.9
3	E	62	MET	2.9
1	C	142	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	130	SER	2.8
3	E	49	PRO	2.8
3	F	133	VAL	2.8
1	C	203	ILE	2.8
3	E	115	LYS	2.8
1	A	198	GLY	2.8
3	E	96	ALA	2.8
1	C	171	VAL	2.8
3	E	70	THR	2.8
3	F	138	LYS	2.8
3	E	203	ILE	2.8
3	F	59	GLY	2.8
1	C	136	SER	2.7
3	E	225	TYR	2.7
1	C	199	THR	2.7
3	E	146	ASP	2.7
3	F	105	ASP	2.7
3	F	127	CYS	2.7
1	C	219	VAL	2.7
1	A	213	THR	2.7
3	F	54	GLN	2.7
1	C	190	VAL	2.7
3	F	33	ASN	2.7
3	E	52	ARG	2.7
3	F	87	ARG	2.7
3	F	108	CYS	2.7
3	F	118	GLN	2.6
1	C	202	TYR	2.6
3	E	262	ASP	2.6
3	F	209	THR	2.6
3	E	102	GLY	2.6
3	E	101	ASP	2.6
3	E	208	ASN	2.6
1	A	211	SER	2.6
3	E	45	SER	2.6
3	F	101	ASP	2.6
3	F	132	GLY	2.6
1	C	222	LYS	2.6
3	F	135	ARG	2.6
1	C	198	GLY	2.6
3	F	49	PRO	2.6
3	F	95	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	267	LYS	2.6
1	C	167	LEU	2.5
3	E	137	ASP	2.5
3	E	48	GLY	2.5
1	C	170	GLY	2.5
3	E	83	PRO	2.5
3	E	76	LEU	2.5
1	A	142	GLY	2.5
1	A	193	PRO	2.5
3	E	68	THR	2.5
3	F	258	ILE	2.5
3	E	157	ASP	2.5
3	E	202	GLN	2.5
1	C	220	GLU	2.4
3	F	112	GLY	2.4
1	A	194	SER	2.4
1	C	201	THR	2.4
1	C	194	SER	2.4
3	E	81	SER	2.4
3	E	98	VAL	2.4
3	F	80	MET	2.4
3	E	192	ALA	2.4
3	F	166	ALA	2.4
3	E	77	LYS	2.4
3	E	267	LYS	2.4
3	E	53	CYS	2.4
3	F	47	ASP	2.3
3	F	259	TYR	2.3
3	F	260	TYR	2.3
1	A	192	VAL	2.3
3	F	53	CYS	2.3
1	A	206	VAL	2.3
1	C	193	PRO	2.3
1	C	143	THR	2.3
3	E	111	GLU	2.3
3	E	198	GLN	2.3
3	E	156	ILE	2.3
3	E	265	PRO	2.3
3	E	41	MET	2.3
3	F	62	MET	2.3
3	E	152	HIS	2.3
3	E	72	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	34	CYS	2.2
1	A	127	PRO	2.2
1	C	144	ALA	2.2
3	E	32	ASP	2.2
1	A	166	ALA	2.2
1	A	222	LYS	2.2
3	E	170	SER	2.2
3	E	210	SER	2.2
1	C	163	ASN	2.2
1	A	221	PRO	2.2
3	F	266	PRO	2.2
3	E	187	HIS	2.2
3	E	184	TYR	2.2
3	F	263	GLU	2.2
3	E	86	ALA	2.2
3	E	93	SER	2.2
3	F	206	ARG	2.1
3	E	79	ARG	2.1
3	F	91	ARG	2.1
3	E	224	TYR	2.1
1	A	218	LYS	2.1
1	C	192	VAL	2.1
3	F	102	GLY	2.1
3	F	104	TYR	2.1
1	A	204	CYS	2.1
3	F	55	CYS	2.1
3	E	193	ALA	2.1
3	F	63	ALA	2.1
3	E	55	CYS	2.0
3	E	94	GLU	2.0
1	C	200	GLN	2.0
3	E	97	LEU	2.0
3	E	257	LEU	2.0
3	E	91	ARG	2.0
3	E	194	VAL	2.0
2	D	121	SER	2.0
3	E	216	ASP	2.0
1	A	214	LYS	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 oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	E	301	14/15	0.58	0.16	87,90,94,101	0
5	NAG	F	301	14/15	0.66	0.15	74,82,87,89	0
4	EDO	B	301	4/4	0.81	0.11	36,38,44,45	0
4	EDO	A	301	4/4	0.84	0.11	32,38,40,42	0
4	EDO	D	301	4/4	0.85	0.13	38,38,40,48	0
4	EDO	C	301	4/4	0.90	0.10	31,37,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.