Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2025 – 08:07 AM EDT

PDB ID	:	9NF6
Title	:	Cg10062 E114N mutant with a covalent hydroxypropionate and acrylate intermediate of the hydration of acetylenecarboxylic acid
Authors	:	Silva, K.; Geiger, J.H.; Draths, K.
Deposited on	:	2025-02-20
Resolution	:	2.63 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

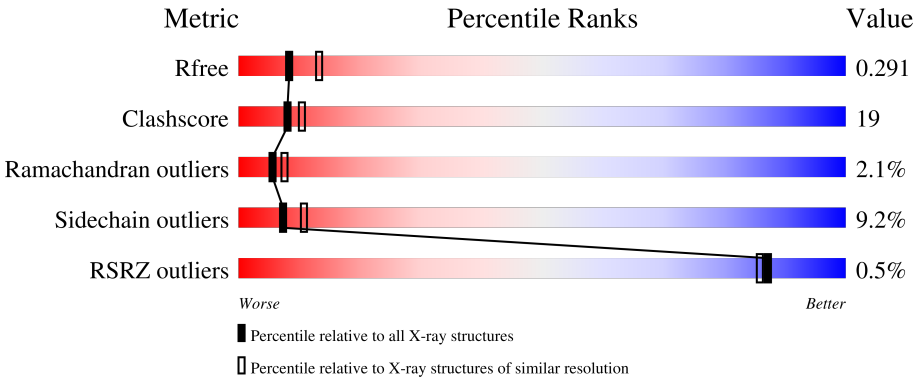
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.63 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}	164625	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

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	148	57% 38%
1	B	148	52% 43%
1	C	148	61% 36%
1	D	148	56% 35% 7%
1	E	148	54% 39% 7%

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Mol	Chain	Length	Quality of chain
1	F	148	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	201	-	-	X	-
3	AKR	B	201	-	X	X	-
4	3OH	C	201	-	X	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7294 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.

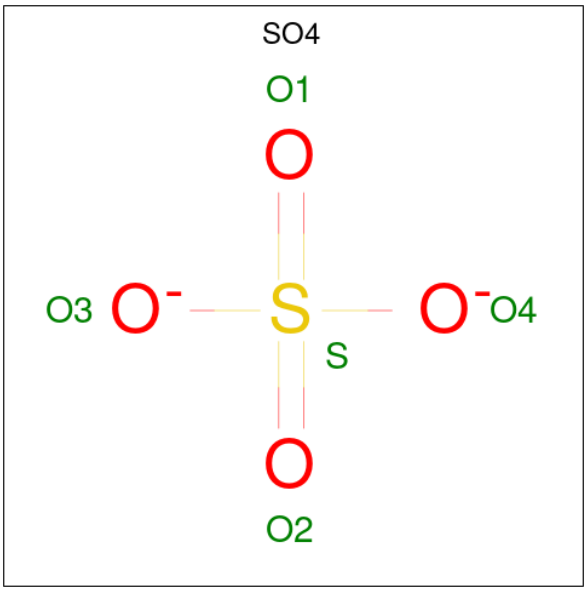
- Molecule 1 is a protein called 4-oxalocrotonate tautomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1204	760	208	233	3			
1	B	147	Total	C	N	O	S	0	0	0
			1195	755	207	230	3			
1	C	147	Total	C	N	O	S	0	0	0
			1195	755	207	230	3			
1	D	146	Total	C	N	O	S	0	0	0
			1189	752	206	228	3			
1	E	148	Total	C	N	O	S	0	0	0
			1204	760	208	233	3			
1	F	147	Total	C	N	O	S	0	0	0
			1195	755	207	230	3			

There are 6 discrepancies between the modelled and reference sequences:

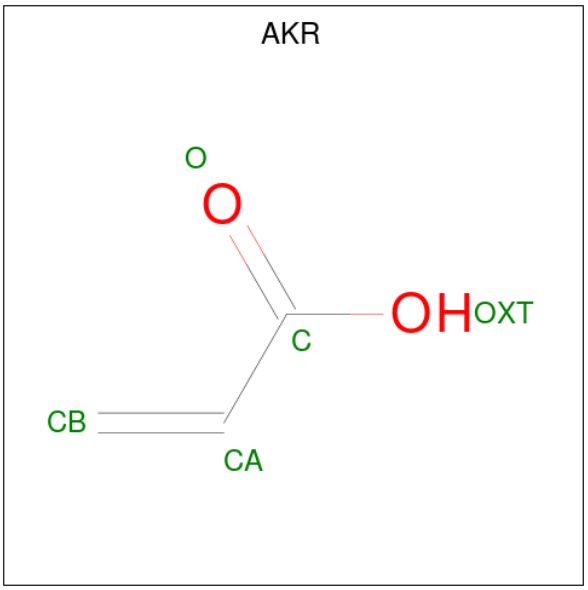
Chain	Residue	Modelled	Actual	Comment	Reference
A	114	ASN	GLU	engineered mutation	UNP A0A0S2T163
B	114	ASN	GLU	engineered mutation	UNP A0A0S2T163
C	114	ASN	GLU	engineered mutation	UNP A0A0S2T163
D	114	ASN	GLU	engineered mutation	UNP A0A0S2T163
E	114	ASN	GLU	engineered mutation	UNP A0A0S2T163
F	114	ASN	GLU	engineered mutation	UNP A0A0S2T163

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



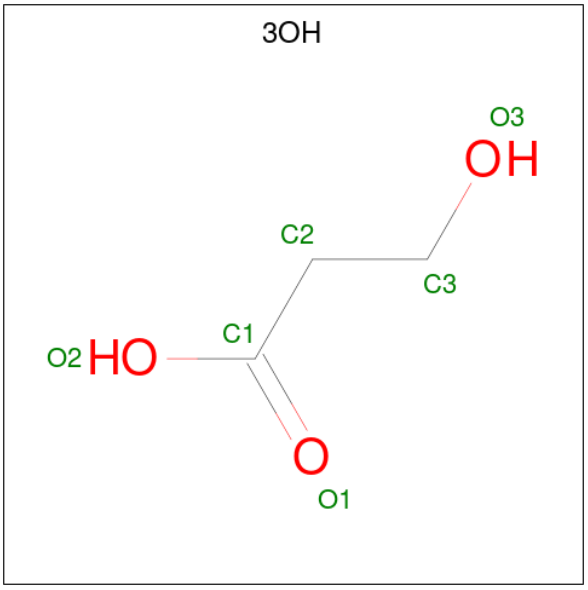
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is ACRYLIC ACID (three-letter code: AKR) (formula: $C_3H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 5 3 2	0	0

- Molecule 4 is 3-HYDROXY-PROPANOIC ACID (three-letter code: 3OH) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

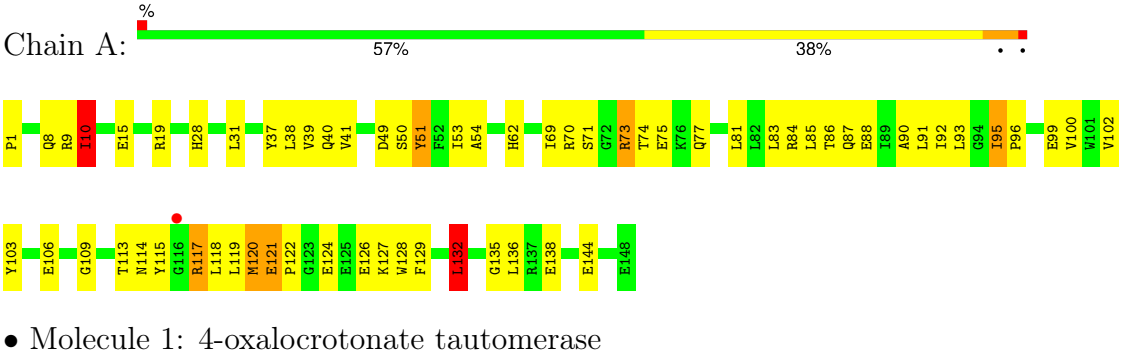
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0
5	B	16	Total O 16 16	0	0
5	C	16	Total O 16 16	0	0
5	D	11	Total O 11 11	0	0
5	E	11	Total O 11 11	0	0
5	F	15	Total O 15 15	0	0

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.

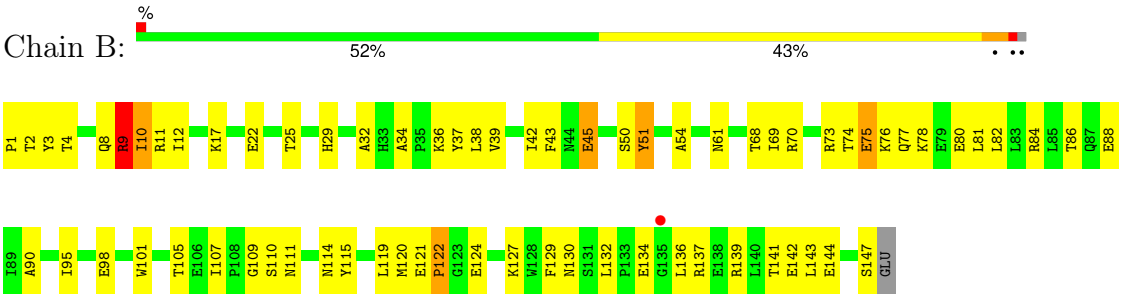
• Molecule 1: 4-oxalocrotonate tautomerase

Chain A:



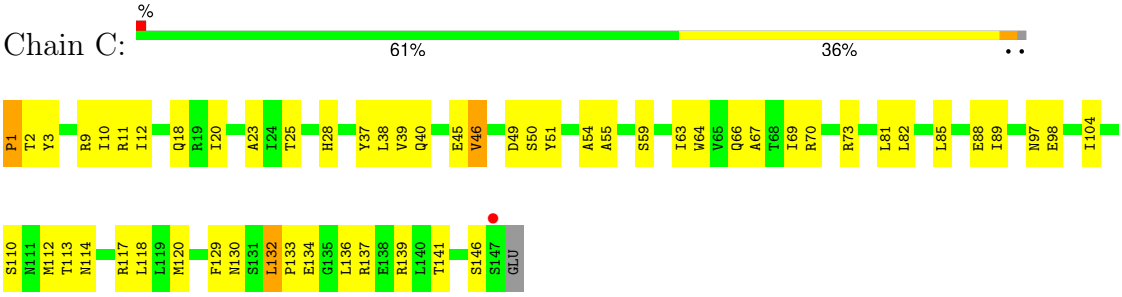
• Molecule 1: 4-oxalocrotonate tautomerase

Chain B:



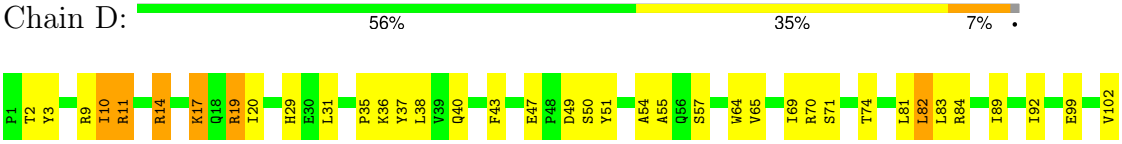
• Molecule 1: 4-oxalocrotonate tautomerase

Chain C:



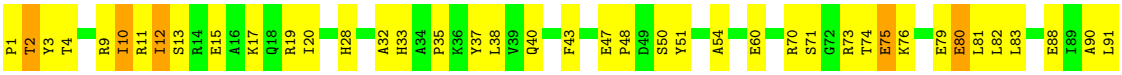
• Molecule 1: 4-oxalocrotonate tautomerase

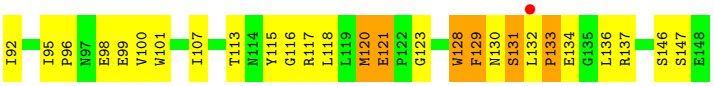
Chain D:



• Molecule 1: 4-oxalocrotonate tautomerase

Chain E:





• Molecule 1: 4-oxalocrotonate tautomerase

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.40Å 88.06Å 79.32Å 90.00° 100.34° 90.00°	Depositor
Resolution (Å)	33.49 – 2.63 33.49 – 2.63	Depositor EDS
% Data completeness (in resolution range)	67.2 (33.49-2.63) 84.2 (33.49-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.194 , 0.293 0.194 , 0.291	Depositor DCC
R_{free} test set	28666 reflections (7.72%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7294	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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: AKR, SO4, 3OH

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	0.49	0/1230	0.69	1/1668 (0.1%)
1	B	0.47	0/1221	0.67	0/1656
1	C	0.46	0/1221	0.69	1/1656 (0.1%)
1	D	0.46	0/1215	0.67	1/1648 (0.1%)
1	E	0.48	0/1230	0.68	0/1668
1	F	0.48	1/1221 (0.1%)	0.67	1/1656 (0.1%)
All	All	0.47	1/7338 (0.0%)	0.68	4/9952 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	33	HIS	C-N	-6.06	1.20	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	143	LEU	CA-CB-CG	6.01	129.12	115.30
1	C	132	LEU	CA-CB-CG	5.25	127.37	115.30
1	D	118	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	132	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	11	ARG	Sidechain

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	1204	0	1181	55	0
1	B	1195	0	1174	55	0
1	C	1195	0	1175	57	0
1	D	1189	0	1170	52	0
1	E	1204	0	1181	50	0
1	F	1195	0	1175	46	0
2	A	5	0	0	2	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
3	B	5	0	1	3	0
4	C	6	0	4	10	0
5	A	12	0	0	3	0
5	B	16	0	0	2	0
5	C	16	0	0	1	0
5	D	11	0	0	0	0
5	E	11	0	0	0	0
5	F	15	0	0	1	0
All	All	7294	0	7061	274	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 19.

All (274) 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:C:1:PRO:H3	4:C:201:3OH:C3	1.28	1.45
1:C:1:PRO:N	4:C:201:3OH:H32	1.31	1.44
1:C:1:PRO:N	4:C:201:3OH:C3	1.84	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:N	3:B:201:AKR:O	1.84	1.08
1:C:1:PRO:N	4:C:201:3OH:H31	1.66	1.07
1:A:74:THR:OG1	1:A:77:GLN:HG3	1.58	1.02
1:C:1:PRO:H2	4:C:201:3OH:C3	1.73	0.92
1:C:1:PRO:H3	4:C:201:3OH:H32	0.88	0.85
1:F:70:ARG:HE	1:F:119:LEU:HD23	1.43	0.84
1:B:70:ARG:HH21	1:B:122:PRO:HA	1.41	0.84
1:C:37:TYR:HA	1:E:54:ALA:HB2	1.61	0.82
1:D:55:ALA:HB1	1:F:22:GLU:HG2	1.64	0.79
1:F:20:ILE:HD11	1:F:93:LEU:HD11	1.66	0.77
1:C:1:PRO:CD	4:C:201:3OH:H31	2.13	0.77
1:C:1:PRO:CA	4:C:201:3OH:H32	2.15	0.76
1:B:86:THR:HG21	1:E:116:GLY:HA2	1.66	0.76
1:C:134:GLU:HA	1:C:137:ARG:HB2	1.68	0.76
1:E:33:HIS:H	1:E:73:ARG:HH12	1.33	0.74
1:C:2:THR:HG22	1:C:40:GLN:HB2	1.69	0.72
1:F:38:LEU:HD22	1:F:114:ASN:HD22	1.54	0.71
1:C:1:PRO:H3	4:C:201:3OH:C2	2.04	0.71
1:F:15:GLU:HG2	1:F:19:ARG:HH22	1.55	0.70
1:A:38:LEU:HD22	5:A:304:HOH:O	1.93	0.69
1:B:43:PHE:HB2	1:C:50:SER:HB3	1.73	0.68
1:C:1:PRO:H2	4:C:201:3OH:H32	1.33	0.68
1:B:50:SER:HB3	1:E:43:PHE:HB2	1.77	0.66
1:C:136:LEU:HD12	1:C:139:ARG:HB3	1.76	0.66
1:A:74:THR:HG1	1:A:77:GLN:HG3	1.60	0.66
1:A:109:GLY:HA3	1:A:120:MET:O	1.95	0.66
1:B:141:THR:HA	1:B:144:GLU:HB3	1.77	0.66
1:A:120:MET:HE1	1:A:127:LYS:HB3	1.79	0.65
1:D:117:ARG:HH21	1:D:133:PRO:HD3	1.61	0.65
1:E:9:ARG:HG2	1:E:10:ILE:HG13	1.79	0.65
1:A:1:PRO:HG3	1:A:28:HIS:CE1	2.32	0.64
1:B:69:ILE:HB	3:B:201:AKR:O	1.97	0.64
1:E:129:PHE:HZ	1:E:137:ARG:HG3	1.62	0.64
1:E:70:ARG:HA	1:E:107:ILE:O	1.97	0.64
1:C:67:ALA:HB3	1:C:104:ILE:HG12	1.80	0.64
1:C:132:LEU:HB3	1:C:137:ARG:HD3	1.79	0.64
1:A:126:GLU:HG3	1:A:129:PHE:HB3	1.80	0.64
1:B:70:ARG:NH1	3:B:201:AKR:OXT	2.31	0.64
1:D:65:VAL:HB	1:D:102:VAL:HG22	1.80	0.64
1:E:11:ARG:HE	1:E:60:GLU:HB3	1.63	0.63
1:B:130:ASN:HB2	5:B:303:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:PRO:HG3	1:E:28:HIS:CD2	2.34	0.63
1:E:132:LEU:HG	1:E:133:PRO:HD2	1.81	0.63
1:B:54:ALA:HB2	1:E:37:TYR:HA	1.81	0.62
1:B:70:ARG:HB3	1:B:122:PRO:HD3	1.82	0.62
1:F:70:ARG:HB2	2:F:201:SO4:O2	2.00	0.62
1:A:113:THR:HG22	1:A:118:LEU:HD12	1.81	0.62
1:C:40:GLN:HG3	1:E:101:TRP:CZ3	2.35	0.62
1:C:1:PRO:HG3	1:C:28:HIS:CD2	2.35	0.62
1:D:54:ALA:HB2	1:F:37:TYR:HA	1.81	0.61
1:E:35:PRO:HD2	1:E:38:LEU:HD22	1.83	0.60
1:B:32:ALA:HA	1:B:77:GLN:NE2	2.16	0.60
1:C:23:ALA:HB1	1:C:88:GLU:OE1	2.01	0.60
1:B:1:PRO:HA	1:B:68:THR:O	2.01	0.60
1:A:70:ARG:HB2	2:A:201:SO4:O2	2.02	0.60
1:E:47:GLU:HB3	1:E:48:PRO:HD2	1.83	0.60
1:A:83:LEU:HD21	1:D:118:LEU:HG	1.83	0.59
1:D:83:LEU:HD21	1:F:118:LEU:HD11	1.84	0.59
1:A:71:SER:HA	1:A:106:GLU:HB3	1.84	0.59
1:C:129:PHE:O	1:C:137:ARG:HD3	2.03	0.59
1:C:9:ARG:HG2	1:C:45:GLU:HB3	1.85	0.59
1:C:12:ILE:HD11	1:C:63:ILE:HD12	1.85	0.59
1:A:95:ILE:HD11	1:A:100:VAL:HG23	1.85	0.58
1:A:129:PHE:O	1:A:132:LEU:HG	2.02	0.58
1:F:1:PRO:HG3	1:F:28:HIS:NE2	2.17	0.58
1:B:115:TYR:HA	1:C:98:GLU:HA	1.86	0.58
1:A:40:GLN:HG3	1:F:53:ILE:HD13	1.85	0.57
1:C:117:ARG:HH21	1:C:133:PRO:HD3	1.69	0.57
1:B:76:LYS:O	1:B:80:GLU:HG3	2.04	0.57
1:F:70:ARG:NE	1:F:119:LEU:HD23	2.18	0.57
1:F:140:LEU:HD13	1:F:143:LEU:HD23	1.85	0.57
1:F:133:PRO:HD2	1:F:136:LEU:HD12	1.86	0.57
1:E:113:THR:HG22	1:E:118:LEU:HD23	1.86	0.57
1:D:132:LEU:HB2	1:D:137:ARG:HB2	1.86	0.57
1:E:131:SER:HB3	1:E:136:LEU:HB2	1.87	0.57
1:A:117:ARG:CZ	1:A:132:LEU:HD22	2.35	0.56
1:E:117:ARG:HH21	1:E:132:LEU:HD12	1.70	0.56
1:D:129:PHE:HA	1:D:132:LEU:HD23	1.86	0.56
1:C:10:ILE:O	1:C:10:ILE:HG22	2.06	0.56
1:F:134:GLU:HA	1:F:137:ARG:NH1	2.21	0.56
1:C:1:PRO:HD2	1:C:38:LEU:O	2.06	0.56
1:B:29:HIS:ND1	1:B:36:LYS:HG3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:THR:HG21	1:D:116:GLY:HA2	1.88	0.55
1:F:70:ARG:HD2	1:F:122:PRO:HD3	1.89	0.55
1:E:90:ALA:HA	1:E:95:ILE:HG12	1.87	0.55
1:C:81:LEU:O	1:C:85:LEU:HG	2.07	0.55
1:B:129:PHE:CZ	1:B:137:ARG:HB2	2.41	0.55
1:D:128:TRP:CE3	1:D:132:LEU:HD21	2.42	0.55
1:F:81:LEU:O	1:F:85:LEU:HG	2.07	0.55
1:C:113:THR:HG23	1:E:82:LEU:HD22	1.89	0.54
1:B:9:ARG:HA	1:B:45:GLU:HB3	1.90	0.54
1:F:1:PRO:HD2	1:F:38:LEU:O	2.06	0.54
1:A:117:ARG:NE	1:A:132:LEU:HD22	2.23	0.54
1:D:89:ILE:HA	1:D:92:ILE:HD12	1.90	0.54
1:D:82:LEU:HG	1:F:113:THR:HG23	1.90	0.54
1:E:129:PHE:CZ	1:E:137:ARG:HG3	2.43	0.54
1:B:124:GLU:OE1	1:B:127:LYS:HD2	2.08	0.53
1:A:70:ARG:HD2	1:A:121:GLU:HA	1.90	0.53
1:B:139:ARG:HA	1:B:142:GLU:OE1	2.09	0.53
1:A:81:LEU:O	1:A:85:LEU:HG	2.09	0.53
1:D:112:MET:HE2	1:D:119:LEU:HD23	1.90	0.53
1:B:12:ILE:HG22	1:B:17:LYS:HG3	1.91	0.52
1:A:117:ARG:NH2	1:A:132:LEU:HB3	2.24	0.52
1:F:7:SER:HB3	1:F:63:ILE:HD13	1.91	0.52
1:B:1:PRO:HG2	1:B:39:VAL:HA	1.93	0.51
1:D:38:LEU:HD23	1:D:70:ARG:HH12	1.74	0.51
1:B:68:THR:HA	1:B:105:THR:O	2.11	0.51
1:C:2:THR:CG2	1:C:40:GLN:HE21	2.24	0.51
1:F:19:ARG:HB3	1:F:92:ILE:HD13	1.92	0.51
1:F:3:TYR:HB2	1:F:41:VAL:HG22	1.92	0.51
1:A:73:ARG:NH1	1:A:122:PRO:HB3	2.26	0.51
1:B:61:ASN:HB3	1:B:95:ILE:HG21	1.93	0.51
1:F:37:TYR:CG	1:F:140:LEU:HD12	2.46	0.51
1:D:71:SER:HB3	1:D:106:GLU:HB2	1.93	0.50
1:E:28:HIS:O	1:E:32:ALA:HB3	2.11	0.50
1:B:34:ALA:HB1	1:B:38:LEU:HD12	1.93	0.50
1:A:69:ILE:HB	2:A:201:SO4:O3	2.12	0.50
1:E:117:ARG:HB2	1:E:128:TRP:NE1	2.26	0.50
1:F:20:ILE:HG23	1:F:89:ILE:HD12	1.94	0.50
1:C:20:ILE:HG23	1:C:89:ILE:HD12	1.93	0.50
1:D:49:ASP:HB2	1:F:14:ARG:HG3	1.93	0.50
1:C:1:PRO:HG3	1:C:28:HIS:NE2	2.27	0.50
1:C:9:ARG:HG3	1:C:46:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:LEU:HD21	1:C:136:LEU:HD23	1.94	0.49
1:E:3:TYR:OH	1:E:81:LEU:HD21	2.13	0.49
1:A:135:GLY:O	1:A:138:GLU:HB2	2.13	0.49
1:D:112:MET:CE	1:D:119:LEU:HD23	2.42	0.49
1:A:73:ARG:CZ	1:A:122:PRO:HB3	2.43	0.49
1:E:120:MET:HG3	1:E:121:GLU:HG2	1.94	0.49
1:E:17:LYS:HG2	1:E:43:PHE:CD2	2.48	0.48
1:E:118:LEU:O	1:E:128:TRP:CD1	2.66	0.48
1:A:124:GLU:OE2	1:A:127:LYS:HD3	2.13	0.48
1:C:130:ASN:HA	1:C:137:ARG:NH1	2.29	0.48
1:C:132:LEU:HD22	1:C:137:ARG:HG2	1.95	0.48
1:F:70:ARG:HB3	1:F:122:PRO:HD3	1.95	0.47
1:F:1:PRO:HB3	1:F:69:ILE:HG22	1.96	0.47
1:A:117:ARG:HB3	5:A:306:HOH:O	2.13	0.47
1:C:2:THR:HG21	1:C:40:GLN:HE21	1.79	0.47
1:A:49:ASP:OD2	1:D:14:ARG:HB3	2.15	0.47
1:E:96:PRO:HD2	1:E:99:GLU:HG3	1.96	0.47
1:B:9:ARG:HB3	1:B:10:ILE:H	1.39	0.47
1:D:133:PRO:HD2	1:D:136:LEU:HD23	1.96	0.47
1:A:129:PHE:HA	1:A:132:LEU:HD21	1.96	0.47
1:D:69:ILE:O	1:D:106:GLU:HA	2.14	0.47
1:A:37:TYR:HA	1:F:54:ALA:HB2	1.97	0.47
1:B:82:LEU:HB3	1:E:113:THR:CG2	2.45	0.47
1:A:40:GLN:HG3	1:F:53:ILE:CD1	2.45	0.47
1:A:113:THR:HG23	1:F:82:LEU:HD22	1.97	0.47
1:F:8:GLN:HB3	5:F:308:HOH:O	2.14	0.47
1:B:3:TYR:OH	1:B:81:LEU:HD21	2.15	0.47
1:D:120:MET:HG2	1:D:124:GLU:OE1	2.15	0.46
1:A:114:ASN:OD1	1:A:119:LEU:HD11	2.15	0.46
1:A:93:LEU:HB2	1:A:95:ILE:HG12	1.96	0.46
1:C:1:PRO:HB3	1:C:69:ILE:HG22	1.96	0.46
1:D:20:ILE:HG23	1:D:89:ILE:HG12	1.97	0.46
1:A:115:TYR:HA	1:F:98:GLU:HA	1.98	0.46
1:B:75:GLU:HA	1:B:78:LYS:HE2	1.98	0.46
1:B:111:ASN:HA	1:C:82:LEU:HD11	1.96	0.46
1:B:90:ALA:HB1	1:B:95:ILE:O	2.16	0.46
1:D:132:LEU:HD12	1:D:136:LEU:CD2	2.46	0.46
1:D:134:GLU:HG2	1:D:135:GLY:N	2.30	0.46
1:A:103:TYR:CE2	1:D:2:THR:HG23	2.50	0.45
1:B:22:GLU:HG2	1:C:55:ALA:HB1	1.97	0.45
1:D:36:LYS:HB2	1:D:144:GLU:OE1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:HD12	1:D:136:LEU:HD21	1.99	0.45
1:E:13:SER:HB2	1:E:15:GLU:OE1	2.15	0.45
1:F:1:PRO:HG3	1:F:28:HIS:CD2	2.51	0.45
1:F:11:ARG:HA	1:F:11:ARG:HD2	1.58	0.45
1:A:53:ILE:HD11	1:A:62:HIS:CE1	2.52	0.45
1:A:103:TYR:CZ	1:D:2:THR:HG23	2.52	0.45
1:E:73:ARG:HD3	1:E:73:ARG:N	2.31	0.45
1:D:70:ARG:HA	1:D:107:ILE:O	2.15	0.45
1:A:93:LEU:O	1:A:95:ILE:HG23	2.16	0.45
1:C:114:ASN:N	1:C:114:ASN:HD22	2.15	0.45
1:D:35:PRO:HG3	1:D:125:GLU:OE2	2.16	0.45
1:E:2:THR:HG22	1:E:40:GLN:NE2	2.32	0.45
1:B:136:LEU:HD22	1:C:98:GLU:HG2	1.98	0.44
1:E:88:GLU:HA	1:E:91:LEU:HD23	1.99	0.44
1:B:70:ARG:HA	1:B:107:ILE:O	2.17	0.44
1:F:114:ASN:HB2	1:F:119:LEU:CD1	2.47	0.44
1:A:1:PRO:HD2	1:A:39:VAL:HA	1.99	0.44
1:A:37:TYR:CD1	1:A:38:LEU:HD23	2.53	0.44
1:B:73:ARG:HE	1:B:73:ARG:HB2	1.53	0.44
1:D:47:GLU:O	1:D:50:SER:HB2	2.18	0.44
1:E:15:GLU:CD	1:E:15:GLU:H	2.21	0.44
1:B:132:LEU:HD23	1:B:136:LEU:HD23	1.99	0.44
1:E:1:PRO:HB2	1:E:3:TYR:CE1	2.53	0.44
1:D:109:GLY:HA3	1:D:120:MET:O	2.18	0.44
1:E:76:LYS:O	1:E:80:GLU:HB2	2.17	0.44
1:B:32:ALA:HA	1:B:77:GLN:HE21	1.81	0.44
1:D:83:LEU:HD21	1:F:118:LEU:CD1	2.46	0.44
1:A:54:ALA:HB2	1:D:37:TYR:HA	2.00	0.43
1:C:118:LEU:HD11	1:E:83:LEU:HG	2.00	0.43
1:B:84:ARG:O	1:B:88:GLU:HG2	2.18	0.43
1:B:98:GLU:HG3	1:E:136:LEU:HD21	1.98	0.43
1:D:99:GLU:OE1	1:D:99:GLU:HA	2.19	0.43
1:C:70:ARG:HB3	1:C:112:MET:HE3	2.01	0.43
1:E:15:GLU:O	1:E:19:ARG:HG3	2.19	0.43
1:A:85:LEU:HD12	1:A:102:VAL:HG11	2.00	0.43
1:B:8:GLN:HG2	1:B:51:TYR:HD2	1.83	0.43
1:B:8:GLN:O	1:B:11:ARG:HB3	2.17	0.43
1:B:98:GLU:HA	1:E:115:TYR:C	2.39	0.43
1:D:64:TRP:HB2	1:F:40:GLN:HE22	1.83	0.43
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.88	0.43
1:D:17:LYS:HG2	1:D:43:PHE:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ARG:HB3	1:C:112:MET:CE	2.49	0.43
1:B:109:GLY:HA3	1:B:120:MET:O	2.19	0.43
1:B:70:ARG:NH2	1:B:122:PRO:HA	2.21	0.42
1:B:98:GLU:OE2	1:E:132:LEU:HD22	2.19	0.42
1:D:31:LEU:HD11	1:D:84:ARG:HD3	2.01	0.42
1:E:131:SER:HB3	1:E:136:LEU:CB	2.49	0.42
1:A:118:LEU:HD11	1:F:82:LEU:HD13	2.00	0.42
1:C:20:ILE:HG12	1:C:89:ILE:HD12	2.01	0.42
1:D:11:ARG:HD2	1:D:11:ARG:O	2.19	0.42
1:E:117:ARG:HB2	1:E:128:TRP:HE1	1.83	0.42
1:F:2:THR:HG23	1:F:40:GLN:HB3	2.01	0.42
1:F:121:GLU:HG3	1:F:122:PRO:HD2	2.00	0.42
1:A:10:ILE:HA	5:A:301:HOH:O	2.18	0.42
1:C:113:THR:HG22	1:C:118:LEU:HG	2.01	0.42
1:E:20:ILE:HG13	1:E:92:ILE:HG21	2.01	0.42
1:A:51:TYR:OH	1:D:40:GLN:NE2	2.52	0.42
1:A:1:PRO:HG3	1:A:28:HIS:ND1	2.34	0.42
1:A:88:GLU:O	1:A:92:ILE:HG13	2.20	0.42
1:B:114:ASN:HB2	1:B:119:LEU:HD21	2.02	0.42
1:C:25:THR:HG23	1:C:39:VAL:HB	2.02	0.42
1:F:7:SER:HB3	1:F:63:ILE:CD1	2.49	0.42
1:A:50:SER:HB3	1:D:43:PHE:HB2	2.02	0.42
1:B:25:THR:HA	1:B:39:VAL:HG11	2.02	0.42
1:B:134:GLU:HA	1:B:137:ARG:HD3	2.01	0.42
1:C:3:TYR:HE2	1:C:85:LEU:HD11	1.84	0.42
1:A:91:LEU:HA	1:A:91:LEU:HD12	1.71	0.42
1:D:128:TRP:O	1:D:131:SER:HB3	2.20	0.42
1:A:96:PRO:HD2	1:A:99:GLU:HG3	2.02	0.42
1:C:46:VAL:HG23	1:C:50:SER:HB2	2.01	0.42
1:B:4:THR:HA	1:B:42:ILE:O	2.20	0.41
1:B:136:LEU:O	1:B:136:LEU:HG	2.20	0.41
1:C:25:THR:HA	1:C:39:VAL:HG11	2.02	0.41
1:D:119:LEU:HD12	1:D:119:LEU:HA	1.48	0.41
1:F:138:GLU:O	1:F:142:GLU:HG3	2.20	0.41
1:D:19:ARG:HA	1:D:19:ARG:HD3	1.76	0.41
1:A:126:GLU:C	1:A:128:TRP:N	2.72	0.41
1:E:100:VAL:C	1:E:101:TRP:HD1	2.23	0.41
1:D:55:ALA:HB1	1:F:22:GLU:CG	2.42	0.41
1:B:37:TYR:HA	1:C:54:ALA:HB2	2.02	0.41
1:D:35:PRO:HD2	1:D:38:LEU:HD22	2.02	0.41
1:B:101:TRP:N	1:B:101:TRP:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ILE:HB	2:D:201:SO4:O2	2.21	0.41
1:A:9:ARG:O	1:A:10:ILE:HG13	2.21	0.41
1:B:1:PRO:HD2	1:B:38:LEU:O	2.21	0.41
1:B:2:THR:HG21	1:C:64:TRP:CH2	2.56	0.41
1:D:132:LEU:CB	1:D:137:ARG:HB2	2.50	0.41
1:C:134:GLU:HA	1:C:137:ARG:CB	2.44	0.41
1:E:131:SER:OG	1:E:137:ARG:HB2	2.21	0.41
1:F:20:ILE:HD11	1:F:93:LEU:CD1	2.44	0.41
1:F:71:SER:HA	1:F:106:GLU:HB3	2.03	0.41
1:C:130:ASN:HA	1:C:137:ARG:CZ	2.51	0.41
1:C:132:LEU:HD23	1:C:133:PRO:HD2	2.03	0.41
1:D:3:TYR:OH	1:D:81:LEU:HD21	2.21	0.41
1:D:9:ARG:CB	1:D:10:ILE:HD12	2.50	0.40
1:E:74:THR:O	1:E:76:LYS:N	2.54	0.40
1:A:90:ALA:HB1	1:A:95:ILE:O	2.21	0.40
1:E:76:LYS:HD3	1:E:76:LYS:HA	1.82	0.40
1:F:11:ARG:HG3	1:F:11:ARG:HH11	1.87	0.40
1:A:41:VAL:HB	1:F:52:PHE:HB2	2.03	0.40
1:C:73:ARG:HD3	5:C:306:HOH:O	2.20	0.40
1:B:25:THR:HG23	1:B:39:VAL:HB	2.02	0.40
5:B:302:HOH:O	1:E:1:PRO:C	2.59	0.40
1:E:75:GLU:HB3	1:E:79:GLU:OE1	2.22	0.40
1:D:113:THR:HG22	1:D:118:LEU:HD23	2.02	0.40
1:D:128:TRP:CZ3	1:D:132:LEU:HD21	2.56	0.40
1:E:12:ILE:HG21	1:E:17:LYS:HG3	2.04	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	146/148 (99%)	132 (90%)	12 (8%)	2 (1%)	9 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	145/148 (98%)	129 (89%)	13 (9%)	3 (2%)	5 7
1	C	145/148 (98%)	133 (92%)	10 (7%)	2 (1%)	9 12
1	D	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	9 12
1	E	146/148 (99%)	127 (87%)	11 (8%)	8 (6%)	1 1
1	F	145/148 (98%)	130 (90%)	14 (10%)	1 (1%)	19 28
All	All	871/888 (98%)	784 (90%)	69 (8%)	18 (2%)	5 7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	ARG
1	D	10	ILE
1	E	10	ILE
1	E	133	PRO
1	E	146	SER
1	E	147	SER
1	F	10	ILE
1	B	10	ILE
1	E	123	GLY
1	A	120	MET
1	C	146	SER
1	D	134	GLU
1	E	75	GLU
1	E	121	GLU
1	A	10	ILE
1	C	120	MET
1	E	130	ASN
1	B	122	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	130/130 (100%)	115 (88%)	15 (12%)	4 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	129/130 (99%)	120 (93%)	9 (7%)	12 20
1	C	129/130 (99%)	118 (92%)	11 (8%)	8 12
1	D	128/130 (98%)	114 (89%)	14 (11%)	5 7
1	E	130/130 (100%)	117 (90%)	13 (10%)	6 8
1	F	129/130 (99%)	120 (93%)	9 (7%)	12 20
All	All	775/780 (99%)	704 (91%)	71 (9%)	7 11

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	10	ILE
1	A	15	GLU
1	A	19	ARG
1	A	51	TYR
1	A	73	ARG
1	A	75	GLU
1	A	84	ARG
1	A	87	GLN
1	A	95	ILE
1	A	117	ARG
1	A	121	GLU
1	A	132	LEU
1	A	136	LEU
1	A	144	GLU
1	B	9	ARG
1	B	45	GLU
1	B	51	TYR
1	B	74	THR
1	B	75	GLU
1	B	110	SER
1	B	121	GLU
1	B	143	LEU
1	B	147	SER
1	C	1	PRO
1	C	11	ARG
1	C	18	GLN
1	C	46	VAL
1	C	49	ASP
1	C	51	TYR

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Mol	Chain	Res	Type
1	C	59	SER
1	C	66	GLN
1	C	97	ASN
1	C	110	SER
1	C	141	THR
1	D	14	ARG
1	D	17	LYS
1	D	19	ARG
1	D	29	HIS
1	D	51	TYR
1	D	57	SER
1	D	74	THR
1	D	82	LEU
1	D	110	SER
1	D	120	MET
1	D	125	GLU
1	D	130	ASN
1	D	137	ARG
1	D	138	GLU
1	E	2	THR
1	E	4	THR
1	E	12	ILE
1	E	50	SER
1	E	51	TYR
1	E	71	SER
1	E	80	GLU
1	E	98	GLU
1	E	120	MET
1	E	128	TRP
1	E	129	PHE
1	E	131	SER
1	E	134	GLU
1	F	51	TYR
1	F	83	LEU
1	F	84	ARG
1	F	97	ASN
1	F	98	GLU
1	F	110	SER
1	F	132	LEU
1	F	140	LEU
1	F	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	62	HIS
1	B	56	GLN
1	C	87	GLN
1	C	97	ASN
1	D	40	GLN
1	E	114	ASN
1	F	40	GLN
1	F	114	ASN

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	$\#\|Z\| > 2$
3	AKR	B	201	1	4,4,4	3.31	3 (75%)	4,4,4	2.76	2 (50%)
2	SO4	F	201	-	4,4,4	0.67	0	6,6,6	0.43	0
2	SO4	D	201	-	4,4,4	0.52	0	6,6,6	1.32	1 (16%)
2	SO4	E	201	-	4,4,4	0.74	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	201	-	4,4,4	0.60	0	6,6,6	0.30	0
4	3OH	C	201	-	5,5,5	2.29	1 (20%)	5,5,5	2.36	3 (60%)

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	3OH	C	201	-	-	2/3/3/3	-
3	AKR	B	201	1	-	2/2/2/2	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	AKR	CA-C	5.37	1.61	1.46
4	C	201	3OH	O3-C3	-4.67	1.18	1.42
3	B	201	AKR	O-C	3.25	1.31	1.23
3	B	201	AKR	CB-CA	2.00	1.40	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	201	AKR	CB-CA-C	-4.66	113.57	121.50
4	C	201	3OH	O3-C3-C2	2.96	122.07	110.96
4	C	201	3OH	O2-C1-C2	2.78	122.78	114.00
2	D	201	SO4	O4-S-O3	-2.50	94.78	108.54
4	C	201	3OH	C3-C2-C1	2.42	116.43	113.11
3	B	201	AKR	OXT-C-CA	2.42	120.77	114.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	AKR	O-C-CA-CB
3	B	201	AKR	OXT-C-CA-CB
4	C	201	3OH	O1-C1-C2-C3
4	C	201	3OH	O2-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	AKR	3	0
2	F	201	SO4	1	0
2	D	201	SO4	1	0
2	A	201	SO4	2	0
4	C	201	3OH	10	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	33:HIS	C	34:ALA	N	1.20

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	148/148 (100%)	-0.28	1 (0%) 84 82	23, 37, 66, 78	0
1	B	147/148 (99%)	-0.15	1 (0%) 84 82	23, 40, 78, 92	0
1	C	147/148 (99%)	-0.07	1 (0%) 84 82	27, 45, 80, 87	0
1	D	146/148 (98%)	-0.12	0 100 100	27, 45, 67, 76	0
1	E	148/148 (100%)	0.12	1 (0%) 84 82	26, 48, 77, 80	0
1	F	147/148 (99%)	-0.17	0 100 100	27, 44, 79, 87	0
All	All	883/888 (99%)	-0.11	4 (0%) 87 86	23, 43, 77, 92	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	SER	2.5
1	E	132	LEU	2.2
1	B	135	GLY	2.1
1	A	116	GLY	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	AKR	B	201	5/5	0.66	0.19	30,42,51,57	0
4	3OH	C	201	6/6	0.80	0.17	30,42,45,47	0
2	SO4	D	201	5/5	0.90	0.11	42,49,51,60	0
2	SO4	E	201	5/5	0.94	0.08	47,49,51,57	0
2	SO4	F	201	5/5	0.97	0.07	48,49,53,53	0
2	SO4	A	201	5/5	0.98	0.05	32,37,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.