



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:43 AM GMT

PDB ID : 2CBQ
Title : CRYSTAL STRUCTURE OF THE NEOCARZINOSTATIN 1TES15 MUTANT BOUND TO TESTOSTERONE HEMISUCCINATE.
Authors : Drevelle, A.; Graille, M.; Heyd, B.; Sorel, I.; Ulryck, N.; Pecorari, F.; Desmadril, M.; Van Tilbeurgh, H.; Minard, P.
Deposited on : 2006-01-06
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

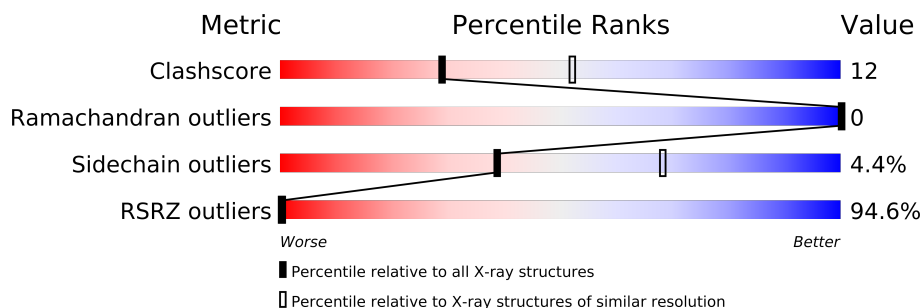
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	114	
1	B	114	
1	C	114	
1	D	114	
1	E	114	
1	F	114	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	1113	-	X
2	SO4	C	1114	-	X
2	SO4	E	1114	-	X
2	SO4	F	1113	-	X
3	TH2	A	1114	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	TH2	A	1115	-	X
3	TH2	B	1116	-	X
3	TH2	B	1117	-	X
3	TH2	C	1115	-	X
3	TH2	D	1114	-	X
3	TH2	E	1115	-	X
3	TH2	F	1114	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5016 atoms, of which 0 are hydrogen and 0 are deuterium.

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 NEOCARZINOSTATIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			773	475	134	162	2			
1	B	113	Total	C	N	O	S	0	0	0
			791	485	139	165	2			
1	C	112	Total	C	N	O	S	0	0	0
			781	479	136	164	2			
1	D	112	Total	C	N	O	S	0	0	0
			781	479	136	164	2			
1	E	112	Total	C	N	O	S	0	0	0
			781	479	136	164	2			
1	F	111	Total	C	N	O	S	0	0	0
			773	475	134	162	2			

There are 42 discrepancies between the modelled and reference sequences:

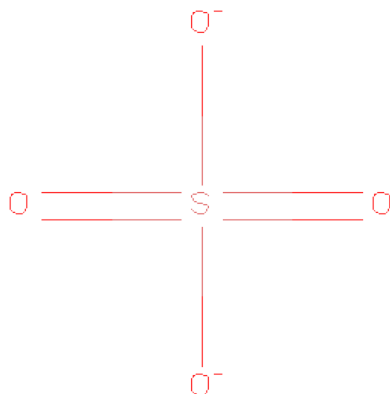
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
A	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
A	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9
A	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
A	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
A	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
A	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9
B	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
B	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
B	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9
B	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
B	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
B	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
B	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9
C	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
C	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
C	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9

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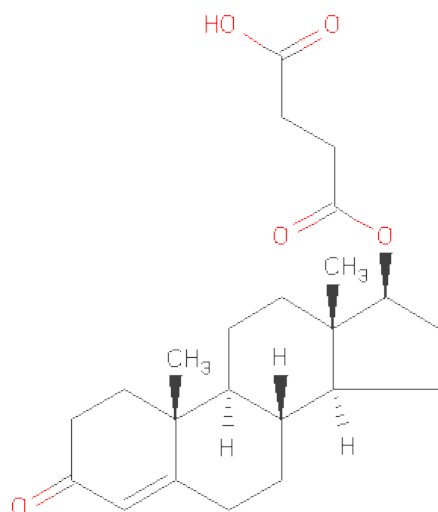
Chain	Residue	Modelled	Actual	Comment	Reference
C	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
C	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
C	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
C	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9
D	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
D	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
D	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9
D	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
D	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
D	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
D	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9
E	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
E	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
E	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9
E	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
E	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
E	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
E	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9
F	33	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
F	35	TYR	GLY	ENGINEERED MUTATION	UNP P0A3R9
F	37	ARG	CYS	ENGINEERED MUTATION	UNP P0A3R9
F	39	ALA	TRP	ENGINEERED MUTATION	UNP P0A3R9
F	45	HIS	LEU	ENGINEERED MUTATION	UNP P0A3R9
F	47	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
F	52	LEU	PHE	ENGINEERED MUTATION	UNP P0A3R9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	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 TESTOSTERONE HEMISUCCINATE (three-letter code: TH2) (formula: $C_{23}H_{32}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 23 5	0	0
3	A	1	Total C O 28 23 5	0	0
3	B	1	Total C O 28 23 5	0	0
3	B	1	Total C O 28 23 5	0	0
3	C	1	Total C O 28 23 5	0	0
3	D	1	Total C O 28 23 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			28	23	5		
3	F	1	Total	C	O	0	0
			28	23	5		

- Molecule 4 is water.

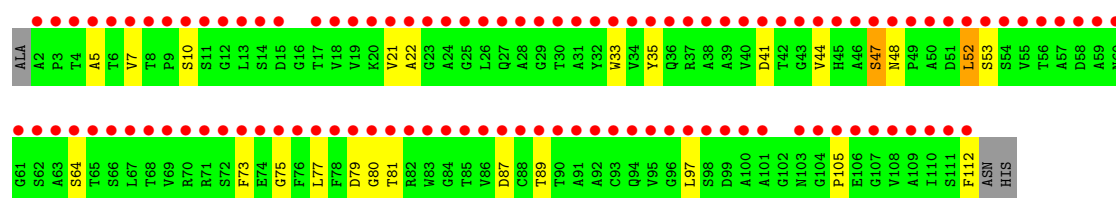
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	17	Total	O	0	0
			17	17		
4	C	17	Total	O	0	0
			17	17		
4	D	17	Total	O	0	0
			17	17		
4	E	14	Total	O	0	0
			14	14		
4	F	7	Total	O	0	0
			7	7		

3 Residue-property plots

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.

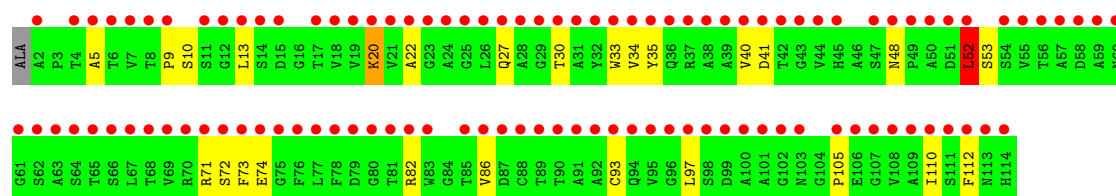
• Molecule 1: NEOCARZINOSTATIN

Chain A: 



• Molecule 1: NEOCARZINOSTATIN

Chain B: 



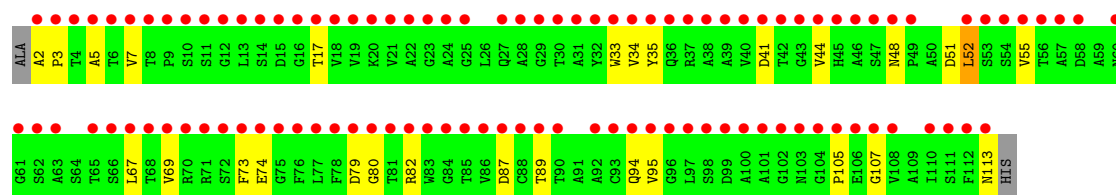
• Molecule 1: NEOCARZINOSTATIN

Chain C: 

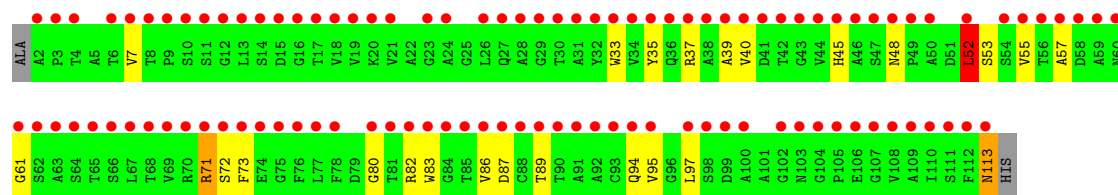


• Molecule 1: NEOCARZINOSTATIN

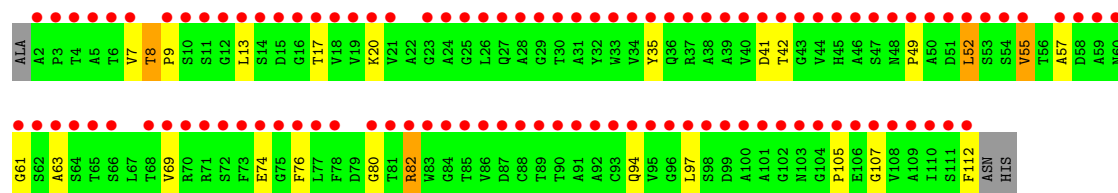
Chain D: 



● Molecule 1: NEOCARZINOSTATIN

Chain E: 

● Molecule 1: NEOCARZINOSTATIN

Chain F: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.98Å 97.83Å 129.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 25.51 – 1.28	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-2.60) 42.5 (25.51-1.28)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 1.28Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.257 0.779 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.55 , 9.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.67$, $\langle L^2 \rangle = 0.55$	Xtriage
Outliers	96 of 78734 reflections (0.122%)	Xtriage
F_o, F_c correlation	0.30	EDS
Total number of atoms	5016	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.30 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8852e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, TH2

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	0.35	0/787	0.64	0/1078
1	B	0.38	0/806	0.64	1/1104 (0.1%)
1	C	0.43	1/795 (0.1%)	0.68	1/1089 (0.1%)
1	D	0.42	1/795 (0.1%)	0.66	1/1089 (0.1%)
1	E	0.41	1/795 (0.1%)	0.67	2/1089 (0.2%)
1	F	0.36	0/787	0.63	0/1078
All	All	0.39	3/4765 (0.1%)	0.66	5/6527 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	113	ASN	CG-OD1	5.51	1.36	1.24
1	D	113	ASN	CG-OD1	5.50	1.36	1.24
1	E	113	ASN	CG-OD1	5.47	1.35	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	113	ASN	OD1-CG-ND2	-6.88	106.08	121.90
1	D	113	ASN	OD1-CG-ND2	-6.88	106.08	121.90
1	C	113	ASN	OD1-CG-ND2	-6.87	106.11	121.90
1	E	52	LEU	CA-CB-CG	5.89	128.84	115.30
1	B	52	LEU	CA-CB-CG	5.47	127.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	773	0	731	21	0
1	B	791	0	744	24	0
1	C	781	0	737	23	0
1	D	781	0	737	16	0
1	E	781	0	737	22	0
1	F	773	0	731	19	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	56	0	62	3	0
3	B	56	0	62	1	0
3	C	28	0	31	0	0
3	D	28	0	31	0	0
3	E	28	0	31	0	0
3	F	28	0	31	0	0
4	A	15	0	0	0	0
4	B	17	0	0	1	0
4	C	17	0	0	2	0
4	D	17	0	0	0	0
4	E	14	0	0	0	0
4	F	7	0	0	0	0
All	All	5016	0	4665	119	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (119) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:37:ARG:HE	1:C:94:GLN:HE21	1.17	0.92
1:D:35:TYR:HB3	1:D:52:LEU:HD23	1.53	0.90
3:A:1115:TH2:H6C2	1:F:20:LYS:HB2	1.53	0.88
3:B:1117:TH2:H6C2	1:C:20:LYS:HB2	1.64	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:37:ARG:NE	1:E:94:GLN:HE21	1.86	0.74
1:E:82:ARG:HG3	1:E:82:ARG:HH11	1.55	0.70
1:B:34:VAL:HG22	1:B:97:LEU:CD1	2.21	0.69
1:E:39:ALA:HA	1:E:45:HIS:HD2	1.58	0.69
1:A:87:ASP:OD2	1:A:89:THR:HB	1.93	0.69
1:A:52:LEU:HD22	1:A:53:SER:H	1.60	0.66
1:C:55:VAL:HG22	1:C:63:ALA:HB1	1.79	0.65
1:C:37:ARG:NE	1:C:94:GLN:HE21	1.92	0.64
1:B:34:VAL:HG22	1:B:97:LEU:HD12	1.79	0.64
1:E:37:ARG:CZ	1:E:94:GLN:HE21	2.12	0.63
1:F:82:ARG:HG2	1:F:82:ARG:NH1	2.14	0.63
1:C:34:VAL:HG23	1:C:54:SER:HA	1.80	0.62
1:E:39:ALA:HA	1:E:45:HIS:CD2	2.34	0.62
1:B:74:GLU:HG3	1:B:82:ARG:NH1	2.15	0.61
1:E:40:VAL:HB	1:E:83:TRP:CZ2	2.34	0.61
1:D:87:ASP:OD2	1:D:89:THR:HB	2.01	0.61
1:B:93:CYS:HB2	4:B:2014:HOH:O	2.00	0.61
1:C:35:TYR:HB3	1:C:52:LEU:HD23	1.84	0.60
1:F:82:ARG:HG2	1:F:82:ARG:HH11	1.69	0.58
1:C:99:ASP:OD2	1:C:103:ASN:HB2	2.04	0.57
1:A:48:ASN:HB2	1:A:73:PHE:CD1	2.39	0.57
1:E:82:ARG:HG3	1:E:82:ARG:NH1	2.20	0.56
1:B:10:SER:O	1:B:110:ILE:HA	2.05	0.56
1:E:52:LEU:HD13	1:E:53:SER:N	2.19	0.56
1:D:7:VAL:HG21	1:D:95:VAL:HB	1.87	0.55
1:C:74:GLU:OE1	1:C:82:ARG:NE	2.40	0.55
1:A:41:ASP:HB3	1:A:44:VAL:HB	1.89	0.54
1:B:34:VAL:HG22	1:B:97:LEU:HD11	1.88	0.54
1:A:52:LEU:HD13	1:A:53:SER:N	2.22	0.54
1:B:48:ASN:HB2	1:B:73:PHE:CD1	2.42	0.54
1:B:20:LYS:NZ	1:B:22:ALA:HB2	2.23	0.54
1:C:58:ASP:HB2	4:C:2010:HOH:O	2.08	0.54
1:D:52:LEU:HD13	1:D:52:LEU:C	2.28	0.53
1:C:48:ASN:HB2	1:C:73:PHE:CD1	2.44	0.53
1:A:33:TRP:CE3	1:A:52:LEU:HD21	2.43	0.53
1:F:82:ARG:HH11	1:F:82:ARG:CG	2.23	0.52
1:F:76:PHE:CE1	1:F:82:ARG:HG3	2.45	0.52
1:F:94:GLN:OE1	1:F:107:GLY:HA3	2.09	0.52
1:C:33:TRP:CE3	1:C:52:LEU:HD11	2.45	0.52
1:C:37:ARG:HH21	1:C:94:GLN:NE2	2.08	0.51
1:E:37:ARG:CZ	1:E:94:GLN:NE2	2.72	0.51
1:A:33:TRP:CZ2	1:C:80:GLY:HA2	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:52:LEU:C	1:A:52:LEU:HD13	2.31	0.51
1:E:48:ASN:HB2	1:E:73:PHE:CD1	2.45	0.51
1:C:37:ARG:HE	1:C:94:GLN:NE2	1.97	0.50
1:C:52:LEU:HD13	1:C:53:SER:N	2.27	0.50
1:D:80:GLY:HA2	1:E:33:TRP:CZ2	2.47	0.50
1:A:52:LEU:HD22	1:A:53:SER:N	2.26	0.49
1:F:97:LEU:HD23	1:F:105:PRO:HG3	1.94	0.49
1:F:7:VAL:HG12	1:F:9:PRO:O	2.13	0.49
1:E:52:LEU:HD13	1:E:52:LEU:C	2.32	0.49
1:B:35:TYR:CD2	1:B:35:TYR:N	2.80	0.48
1:A:5:ALA:HB2	1:A:105:PRO:HG3	1.94	0.48
1:B:72:SER:HA	1:B:86:VAL:O	2.13	0.48
1:E:87:ASP:OD2	1:E:89:THR:HB	2.14	0.48
1:E:7:VAL:HG21	1:E:95:VAL:HB	1.96	0.48
1:E:35:TYR:CD2	1:E:35:TYR:N	2.82	0.48
1:A:33:TRP:HE3	1:A:52:LEU:HD21	1.78	0.47
1:A:33:TRP:CH2	1:C:80:GLY:HA2	2.50	0.47
1:F:57:ALA:HB1	1:F:61:GLY:HA2	1.97	0.47
1:C:52:LEU:C	1:C:52:LEU:HD13	2.36	0.46
1:A:47:SER:HB2	3:A:1114:TH2:O3	2.15	0.46
1:B:52:LEU:HD22	1:B:53:SER:N	2.31	0.46
1:E:71:ARG:HH21	1:E:71:ARG:HB2	1.80	0.45
1:A:77:LEU:HD12	1:A:81:THR:HB	1.97	0.45
1:B:40:VAL:O	1:B:41:ASP:HB2	2.15	0.45
1:C:55:VAL:CG2	1:C:63:ALA:HB1	2.46	0.45
1:B:27:GLN:O	1:B:30:THR:HB	2.16	0.45
1:D:34:VAL:HG12	1:D:67:LEU:HD22	1.98	0.45
1:A:7:VAL:O	1:A:10:SER:HB3	2.15	0.45
1:F:41:ASP:OD1	1:F:42:THR:N	2.47	0.45
1:B:112:PHE:CD1	1:B:112:PHE:N	2.84	0.45
1:D:74:GLU:OE1	1:D:82:ARG:NE	2.37	0.45
1:D:5:ALA:HB2	1:D:105:PRO:HG3	1.99	0.44
1:A:80:GLY:HA2	1:C:33:TRP:CZ2	2.53	0.44
1:A:21:VAL:O	1:A:64:SER:HA	2.17	0.44
1:E:57:ALA:HB1	1:E:61:GLY:HA2	1.99	0.44
1:B:52:LEU:HD22	1:B:53:SER:H	1.82	0.44
1:B:33:TRP:CE3	1:B:52:LEU:HD21	2.53	0.43
1:F:8:THR:HA	1:F:9:PRO:C	2.37	0.43
1:C:7:VAL:HG12	1:C:9:PRO:O	2.17	0.43
1:E:48:ASN:HB2	1:E:73:PHE:CG	2.54	0.43
1:D:33:TRP:CZ2	1:E:80:GLY:HA2	2.54	0.43
1:B:35:TYR:HB3	1:B:52:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:48:ASN:ND2	1:D:51:ASP:HB2	2.34	0.43
1:E:37:ARG:NH1	1:E:45:HIS:ND1	2.66	0.43
1:B:33:TRP:CZ3	1:B:52:LEU:HD11	2.54	0.43
1:A:112:PHE:CD1	1:A:112:PHE:N	2.86	0.43
1:D:41:ASP:HB3	1:D:44:VAL:CG2	2.49	0.43
1:A:47:SER:O	1:A:75:GLY:HA2	2.19	0.42
1:E:72:SER:HA	1:E:86:VAL:O	2.19	0.42
1:C:36:GLN:HB2	4:C:2005:HOH:O	2.19	0.42
1:B:20:LYS:HZ3	1:B:22:ALA:HB2	1.84	0.42
1:C:82:ARG:HH22	1:C:84:GLY:HA2	1.85	0.42
1:C:5:ALA:HA	1:C:22:ALA:O	2.19	0.42
1:B:97:LEU:HB3	1:B:105:PRO:HD2	2.02	0.41
1:B:9:PRO:HG2	1:B:13:LEU:CD2	2.50	0.41
1:F:49:PRO:HA	1:F:52:LEU:HB2	2.02	0.41
1:E:82:ARG:CG	1:E:82:ARG:NH1	2.83	0.41
1:F:17:THR:O	1:F:69:VAL:HG22	2.20	0.41
1:F:74:GLU:CD	1:F:82:ARG:NH1	2.73	0.41
1:F:9:PRO:HG2	1:F:13:LEU:CD2	2.50	0.41
1:D:2:ALA:HA	1:D:3:PRO:HD3	1.89	0.41
1:B:5:ALA:HB2	1:B:105:PRO:HG3	2.03	0.41
1:F:55:VAL:HG22	1:F:63:ALA:HB1	2.03	0.41
1:A:5:ALA:HA	1:A:22:ALA:O	2.20	0.41
1:D:94:GLN:OE1	1:D:107:GLY:HA3	2.21	0.41
1:D:17:THR:O	1:D:69:VAL:HG22	2.20	0.41
1:D:48:ASN:HB2	1:D:73:PHE:CD1	2.56	0.41
1:D:35:TYR:N	1:D:35:TYR:CD2	2.88	0.41
1:F:112:PHE:N	1:F:112:PHE:CD1	2.89	0.41
1:F:35:TYR:HB3	1:F:52:LEU:HD23	2.02	0.40
1:B:33:TRP:O	1:B:97:LEU:HA	2.20	0.40
1:A:35:TYR:CD2	3:A:1114:TH2:H6C1	2.57	0.40
1:B:33:TRP:CZ2	1:F:80:GLY:HA2	2.57	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	109/114 (96%)	106 (97%)	3 (3%)	0	100	100
1	B	111/114 (97%)	107 (96%)	4 (4%)	0	100	100
1	C	110/114 (96%)	104 (94%)	6 (6%)	0	100	100
1	D	110/114 (96%)	105 (96%)	5 (4%)	0	100	100
1	E	110/114 (96%)	107 (97%)	3 (3%)	0	100	100
1	F	109/114 (96%)	105 (96%)	4 (4%)	0	100	100
All	All	659/684 (96%)	634 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	79/81 (98%)	75 (95%)	4 (5%)	33	60
1	B	81/81 (100%)	78 (96%)	3 (4%)	45	75
1	C	80/81 (99%)	78 (98%)	2 (2%)	60	86
1	D	80/81 (99%)	77 (96%)	3 (4%)	44	74
1	E	80/81 (99%)	75 (94%)	5 (6%)	25	49
1	F	79/81 (98%)	75 (95%)	4 (5%)	33	60
All	All	479/486 (99%)	458 (96%)	21 (4%)	39	68

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	52	LEU
1	A	79	ASP
1	A	97	LEU
1	B	20	LYS
1	B	52	LEU
1	B	71	ARG
1	C	55	VAL
1	C	113	ASN

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Mol	Chain	Res	Type
1	D	52	LEU
1	D	55	VAL
1	D	79	ASP
1	E	52	LEU
1	E	55	VAL
1	E	71	ARG
1	E	97	LEU
1	E	113	ASN
1	F	8	THR
1	F	52	LEU
1	F	55	VAL
1	F	82	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	94	GLN
1	C	94	GLN
1	D	45	HIS
1	E	94	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1113	-	4,4,4	0.27	0	6,6,6	0.08	0
3	TH2	A	1114	-	31,31,31	1.47	6 (19%)	48,48,48	1.95	13 (27%)
3	TH2	A	1115	-	31,31,31	1.56	7 (22%)	48,48,48	1.94	12 (25%)
2	SO4	B	1115	-	4,4,4	0.32	0	6,6,6	0.11	0
3	TH2	B	1116	-	31,31,31	1.52	6 (19%)	48,48,48	1.89	11 (22%)
3	TH2	B	1117	-	31,31,31	1.57	7 (22%)	48,48,48	1.99	11 (22%)
2	SO4	C	1114	-	4,4,4	0.29	0	6,6,6	0.13	0
3	TH2	C	1115	-	31,31,31	1.50	6 (19%)	48,48,48	1.90	11 (22%)
3	TH2	D	1114	-	31,31,31	1.55	8 (25%)	48,48,48	1.94	11 (22%)
2	SO4	E	1114	-	4,4,4	0.27	0	6,6,6	0.10	0
3	TH2	E	1115	-	31,31,31	1.48	7 (22%)	48,48,48	1.96	12 (25%)
2	SO4	F	1113	-	4,4,4	0.26	0	6,6,6	0.11	0
3	TH2	F	1114	-	31,31,31	1.48	7 (22%)	48,48,48	1.91	11 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1113	-	-	0/0/0/0	0/0/0/0
3	TH2	A	1114	-	-	0/9/67/67	0/0/4/4
3	TH2	A	1115	-	-	0/9/67/67	0/0/4/4
2	SO4	B	1115	-	-	0/0/0/0	0/0/0/0
3	TH2	B	1116	-	-	0/9/67/67	0/0/4/4
3	TH2	B	1117	-	-	0/9/67/67	0/0/4/4
2	SO4	C	1114	-	-	0/0/0/0	0/0/0/0
3	TH2	C	1115	-	-	0/9/67/67	0/0/4/4
3	TH2	D	1114	-	-	1/9/67/67	0/0/4/4
2	SO4	E	1114	-	-	0/0/0/0	0/0/0/0
3	TH2	E	1115	-	-	0/9/67/67	0/0/4/4
2	SO4	F	1113	-	-	0/0/0/0	0/0/0/0
3	TH2	F	1114	-	-	0/9/67/67	0/0/4/4

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1114	TH2	C10-C5	2.95	1.59	1.52
3	D	1114	TH2	C10-C5	2.87	1.59	1.52
3	B	1117	TH2	C10-C5	2.78	1.59	1.52
3	E	1115	TH2	C16-C17	2.76	1.59	1.53
3	C	1115	TH2	C10-C5	2.75	1.59	1.52
3	A	1115	TH2	C4-C5	2.74	1.38	1.34
3	B	1116	TH2	C10-C5	2.62	1.58	1.52
3	B	1117	TH2	C4-C5	2.56	1.37	1.34
3	A	1115	TH2	C16-C17	2.54	1.59	1.53
3	B	1116	TH2	O17-C17	-2.53	1.41	1.46
3	A	1115	TH2	C10-C5	2.51	1.58	1.52
3	D	1114	TH2	C16-C17	2.48	1.59	1.53
3	D	1114	TH2	C11-C9	2.48	1.58	1.53
3	B	1117	TH2	C16-C17	2.46	1.59	1.53
3	B	1116	TH2	C16-C17	2.41	1.58	1.53
3	A	1114	TH2	O17-C17	-2.40	1.41	1.46
3	E	1115	TH2	C4-C5	2.39	1.37	1.34
3	A	1115	TH2	C1-C10	2.38	1.58	1.54
3	E	1115	TH2	C8-C9	2.33	1.58	1.53
3	F	1114	TH2	C10-C5	2.33	1.58	1.52
3	D	1114	TH2	C7-C8	2.32	1.57	1.53
3	B	1117	TH2	C8-C9	2.31	1.58	1.53
3	B	1117	TH2	C11-C9	2.31	1.58	1.53
3	E	1115	TH2	O17-C17	-2.30	1.42	1.46
3	F	1114	TH2	C16-C17	2.28	1.58	1.53
3	C	1115	TH2	C11-C9	2.27	1.58	1.53
3	A	1114	TH2	C11-C9	2.26	1.57	1.53
3	F	1114	TH2	C4-C5	2.25	1.37	1.34
3	B	1117	TH2	C7-C8	2.23	1.57	1.53
3	C	1115	TH2	C4-C5	2.23	1.37	1.34
3	F	1114	TH2	C7-C8	2.23	1.57	1.53
3	F	1114	TH2	O17-C17	-2.22	1.42	1.46
3	A	1115	TH2	C8-C9	2.22	1.58	1.53
3	D	1114	TH2	C8-C9	2.21	1.58	1.53
3	E	1115	TH2	C10-C5	2.20	1.57	1.52
3	B	1116	TH2	C11-C9	2.18	1.57	1.53
3	B	1116	TH2	O17-C20	-2.18	1.27	1.34
3	D	1114	TH2	C1-C10	2.17	1.58	1.54
3	D	1114	TH2	C4-C5	2.16	1.37	1.34
3	C	1115	TH2	O17-C17	-2.14	1.42	1.46
3	A	1115	TH2	C13-C17	2.14	1.57	1.53
3	E	1115	TH2	O17-C20	-2.14	1.27	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1115	TH2	C1-C10	2.14	1.58	1.54
3	C	1115	TH2	C16-C17	2.10	1.58	1.53
3	F	1114	TH2	C10-C9	2.09	1.60	1.56
3	C	1115	TH2	O3-C3	-2.08	1.19	1.23
3	A	1115	TH2	C11-C9	2.07	1.57	1.53
3	F	1114	TH2	C1-C10	2.06	1.58	1.54
3	A	1114	TH2	O17-C20	-2.06	1.27	1.34
3	A	1114	TH2	C8-C9	2.06	1.57	1.53
3	A	1114	TH2	C16-C17	2.05	1.58	1.53
3	B	1116	TH2	C4-C5	2.04	1.37	1.34
3	B	1117	TH2	O3-C3	-2.04	1.19	1.23
3	D	1114	TH2	O17-C17	-2.00	1.42	1.46

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1115	TH2	O17-C17-C16	5.90	125.74	111.03
3	B	1117	TH2	O17-C17-C16	5.51	124.76	111.03
3	A	1115	TH2	O17-C17-C16	5.27	124.15	111.03
3	F	1114	TH2	O17-C17-C16	5.25	124.12	111.03
3	B	1116	TH2	O17-C17-C16	5.22	124.05	111.03
3	D	1114	TH2	O17-C17-C16	5.09	123.71	111.03
3	A	1114	TH2	O17-C17-C13	5.03	123.53	111.20
3	D	1114	TH2	O17-C17-C13	4.99	123.42	111.20
3	F	1114	TH2	O17-C17-C13	4.82	123.01	111.20
3	C	1115	TH2	O17-C17-C16	4.81	123.02	111.03
3	A	1115	TH2	O17-C17-C13	4.72	122.76	111.20
3	A	1114	TH2	O17-C17-C16	4.71	122.78	111.03
3	B	1117	TH2	C17-O17-C20	4.68	128.13	118.04
3	B	1117	TH2	O17-C17-C13	4.66	122.62	111.20
3	C	1115	TH2	O17-C17-C13	4.63	122.54	111.20
3	E	1115	TH2	C17-O17-C20	4.59	127.95	118.04
3	E	1115	TH2	C11-C9-C10	-4.47	106.89	113.08
3	A	1115	TH2	C17-O17-C20	4.30	127.33	118.04
3	B	1116	TH2	O17-C17-C13	4.28	121.67	111.20
3	C	1115	TH2	C17-O17-C20	4.25	127.20	118.04
3	B	1116	TH2	C11-C9-C10	-4.15	107.32	113.08
3	B	1117	TH2	C11-C9-C10	-4.12	107.37	113.08
3	D	1114	TH2	C11-C9-C10	-4.11	107.38	113.08
3	A	1114	TH2	C11-C9-C10	-4.10	107.40	113.08
3	C	1115	TH2	C11-C9-C10	-4.08	107.41	113.08
3	A	1115	TH2	C11-C9-C10	-4.08	107.42	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1114	TH2	C12-C11-C9	-4.06	106.36	113.15
3	F	1114	TH2	C11-C9-C10	-4.03	107.50	113.08
3	B	1116	TH2	C17-O17-C20	3.95	126.56	118.04
3	B	1117	TH2	C12-C11-C9	-3.93	106.58	113.15
3	A	1114	TH2	C17-O17-C20	3.84	126.33	118.04
3	F	1114	TH2	C17-O17-C20	3.81	126.27	118.04
3	A	1115	TH2	C12-C11-C9	-3.81	106.78	113.15
3	A	1114	TH2	C12-C11-C9	-3.80	106.79	113.15
3	D	1114	TH2	C17-O17-C20	3.80	126.24	118.04
3	F	1114	TH2	C12-C11-C9	-3.75	106.89	113.15
3	E	1115	TH2	C12-C11-C9	-3.72	106.93	113.15
3	E	1115	TH2	O17-C17-C13	3.59	120.00	111.20
3	B	1116	TH2	C12-C11-C9	-3.57	107.19	113.15
3	C	1115	TH2	C12-C11-C9	-3.45	107.39	113.15
3	A	1114	TH2	O17-C20-O20	3.08	131.89	123.65
3	C	1115	TH2	O17-C20-O20	3.00	131.69	123.65
3	E	1115	TH2	O17-C20-O20	2.95	131.55	123.65
3	B	1117	TH2	O17-C20-O20	2.91	131.45	123.65
3	A	1115	TH2	C16-C17-C13	-2.87	102.00	105.20
3	B	1117	TH2	C16-C17-C13	-2.84	102.03	105.20
3	B	1116	TH2	O17-C20-O20	2.82	131.21	123.65
3	C	1115	TH2	C16-C17-C13	-2.76	102.12	105.20
3	A	1115	TH2	O17-C20-O20	2.71	130.91	123.65
3	D	1114	TH2	C16-C17-C13	-2.70	102.19	105.20
3	F	1114	TH2	C16-C17-C13	-2.68	102.21	105.20
3	A	1114	TH2	C16-C17-C13	-2.68	102.22	105.20
3	E	1115	TH2	C16-C17-C13	-2.66	102.24	105.20
3	B	1117	TH2	C18-C13-C14	2.64	117.03	111.76
3	F	1114	TH2	O17-C20-O20	2.60	130.62	123.65
3	A	1114	TH2	C9-C10-C5	-2.59	105.64	109.67
3	F	1114	TH2	C18-C13-C14	2.56	116.88	111.76
3	B	1116	TH2	C16-C17-C13	-2.53	102.38	105.20
3	D	1114	TH2	C18-C13-C14	2.52	116.81	111.76
3	D	1114	TH2	O17-C20-O20	2.52	130.41	123.65
3	A	1115	TH2	O3-C3-C2	2.44	125.25	121.58
3	A	1115	TH2	C9-C10-C5	-2.43	105.88	109.67
3	A	1114	TH2	C22-C21-C23	-2.43	109.02	113.53
3	A	1114	TH2	O20-C20-C22	-2.41	113.85	123.78
3	A	1115	TH2	C18-C13-C14	2.41	116.57	111.76
3	B	1117	TH2	O20-C20-C22	-2.40	113.90	123.78
3	F	1114	TH2	O20-C20-C22	-2.38	113.96	123.78
3	D	1114	TH2	O20-C20-C22	-2.34	114.11	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1114	TH2	C9-C10-C5	-2.32	106.06	109.67
3	E	1115	TH2	O3-C3-C2	2.30	125.04	121.58
3	B	1116	TH2	O20-C20-C22	-2.29	114.33	123.78
3	C	1115	TH2	O3-C3-C2	2.28	125.01	121.58
3	C	1115	TH2	C9-C10-C5	-2.27	106.13	109.67
3	E	1115	TH2	C9-C10-C5	-2.23	106.19	109.67
3	A	1115	TH2	O20-C20-C22	-2.22	114.62	123.78
3	B	1117	TH2	C9-C10-C5	-2.20	106.25	109.67
3	C	1115	TH2	O20-C20-C22	-2.19	114.74	123.78
3	E	1115	TH2	O20-C20-C22	-2.18	114.77	123.78
3	A	1114	TH2	C18-C13-C14	2.16	116.08	111.76
3	D	1114	TH2	O3-C3-C2	2.16	124.83	121.58
3	C	1115	TH2	C15-C16-C17	2.13	108.30	104.84
3	F	1114	TH2	O3-C3-C2	2.12	124.77	121.58
3	E	1115	TH2	C18-C13-C14	2.12	115.99	111.76
3	B	1116	TH2	C18-C13-C14	2.11	115.98	111.76
3	A	1114	TH2	C1-C10-C9	2.09	111.38	108.60
3	A	1114	TH2	O3-C3-C2	2.09	124.72	121.58
3	A	1115	TH2	C1-C10-C9	2.07	111.36	108.60
3	E	1115	TH2	C6-C7-C8	-2.06	108.26	111.71
3	B	1117	TH2	O3-C3-C2	2.03	124.63	121.58
3	B	1116	TH2	C15-C16-C17	2.02	108.13	104.84
3	F	1114	TH2	C9-C10-C5	-2.01	106.54	109.67
3	B	1116	TH2	C9-C10-C5	-2.01	106.55	109.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1114	TH2	C20-O17-C17-C16

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	111/114 (97%)	10.92	109 (98%) 0 0	17, 27, 36, 45	0
1	B	113/114 (99%)	9.64	106 (93%) 0 0	13, 24, 35, 46	0
1	C	112/114 (98%)	10.74	105 (93%) 0 0	16, 25, 36, 50	0
1	D	112/114 (98%)	10.05	105 (93%) 0 0	16, 24, 40, 49	0
1	E	112/114 (98%)	9.98	104 (92%) 0 0	18, 30, 45, 56	0
1	F	111/114 (97%)	11.99	106 (95%) 0 0	17, 31, 45, 50	0
All	All	671/684 (98%)	10.55	635 (94%) 0 0	13, 27, 42, 56	0

All (635) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	SER	50.1
1	B	57	ALA	50.0
1	F	5	ALA	49.9
1	A	2	ALA	47.8
1	D	101	ALA	47.0
1	F	105	PRO	45.7
1	A	91	ALA	44.3
1	E	2	ALA	42.7
1	F	100	ALA	42.1
1	C	100	ALA	42.0
1	F	60	ASN	40.3
1	F	84	GLY	40.0
1	E	29	GLY	39.1
1	C	2	ALA	37.4
1	D	39	ALA	36.0
1	F	108	VAL	35.7
1	C	61	GLY	35.1
1	E	49	PRO	35.1
1	F	57	ALA	34.8

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Mol	Chain	Res	Type	RSRZ
1	A	45	HIS	34.0
1	A	80	GLY	33.8
1	C	92	ALA	33.2
1	E	89	THR	32.3
1	D	90	THR	32.2
1	B	39	ALA	32.1
1	C	18	VAL	32.0
1	C	94	GLN	31.6
1	D	47	SER	31.4
1	F	9	PRO	31.1
1	D	75	GLY	30.5
1	B	5	ALA	30.1
1	E	34	VAL	29.9
1	F	42	THR	29.9
1	A	96	GLY	29.8
1	D	84	GLY	29.3
1	C	63	ALA	29.2
1	C	101	ALA	28.3
1	C	47	SER	28.0
1	C	12	GLY	27.8
1	B	107	GLY	27.8
1	F	50	ALA	27.5
1	A	90	THR	27.5
1	A	62	SER	27.2
1	F	109	ALA	27.2
1	A	69	VAL	27.1
1	D	100	ALA	27.0
1	C	44	VAL	26.9
1	E	26	LEU	26.7
1	E	112	PHE	25.4
1	B	89	THR	25.4
1	A	68	THR	25.4
1	F	101	ALA	25.4
1	D	32	TYR	25.3
1	B	44	VAL	24.9
1	E	21	VAL	24.9
1	B	106	GLU	24.8
1	E	15	ASP	24.7
1	C	109	ALA	24.7
1	A	61	GLY	24.6
1	A	3	PRO	24.4
1	B	15	ASP	24.4

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Mol	Chain	Res	Type	RSRZ
1	C	17	THR	23.9
1	D	40	VAL	23.9
1	E	91	ALA	23.1
1	D	27	GLN	22.6
1	F	23	GLY	22.4
1	D	52	LEU	22.2
1	F	43	GLY	22.1
1	D	24	ALA	21.7
1	E	44	VAL	21.5
1	D	103	ASN	21.3
1	D	112	PHE	21.2
1	A	63	ALA	20.9
1	D	95	VAL	20.8
1	A	104	GLY	20.7
1	F	55	VAL	20.3
1	F	89	THR	20.0
1	A	92	ALA	19.9
1	F	107	GLY	19.8
1	B	4	THR	19.7
1	B	20	LYS	19.5
1	C	10	SER	19.5
1	B	59	ALA	19.4
1	B	102	GLY	19.3
1	A	41	ASP	19.3
1	E	7	VAL	19.1
1	D	14	SER	19.1
1	A	84	GLY	19.0
1	F	2	ALA	18.9
1	F	91	ALA	18.9
1	F	111	SER	18.8
1	F	19	VAL	18.7
1	B	11	SER	18.7
1	E	39	ALA	18.7
1	C	48	ASN	18.7
1	A	98	SER	18.6
1	C	65	THR	18.6
1	D	48	ASN	18.6
1	F	102	GLY	18.6
1	B	109	ALA	18.5
1	E	59	ALA	18.5
1	A	108	VAL	18.2
1	C	9	PRO	18.2

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Mol	Chain	Res	Type	RSRZ
1	E	60	ASN	18.1
1	F	34	VAL	18.1
1	C	32	TYR	18.0
1	D	28	ALA	17.9
1	E	90	THR	17.9
1	B	114	HIS	17.9
1	C	91	ALA	17.8
1	E	36	GLN	17.7
1	C	21	VAL	17.6
1	F	59	ALA	17.4
1	E	99	ASP	17.4
1	D	25	GLY	17.3
1	A	106	GLU	17.2
1	F	88	CYS	17.2
1	F	54	SER	17.1
1	B	93	CYS	17.1
1	D	19	VAL	17.1
1	F	6	THR	17.0
1	D	2	ALA	16.9
1	B	51	ASP	16.9
1	B	14	SER	16.8
1	A	109	ALA	16.7
1	D	38	ALA	16.7
1	E	111	SER	16.7
1	E	80	GLY	16.5
1	F	90	THR	16.5
1	F	99	ASP	16.5
1	B	9	PRO	16.4
1	A	43	GLY	16.1
1	C	72	SER	16.1
1	A	73	PHE	16.1
1	B	37	ARG	16.1
1	C	88	CYS	16.0
1	B	113	ASN	15.9
1	C	20	LYS	15.8
1	A	46	ALA	15.7
1	A	89	THR	15.6
1	D	72	SER	15.6
1	E	77	LEU	15.6
1	F	25	GLY	15.5
1	B	73	PHE	15.4
1	D	93	CYS	15.3

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Mol	Chain	Res	Type	RSRZ
1	C	26	LEU	15.0
1	E	67	LEU	14.9
1	B	32	TYR	14.8
1	D	41	ASP	14.8
1	E	19	VAL	14.7
1	C	40	VAL	14.7
1	A	29	GLY	14.6
1	F	21	VAL	14.5
1	C	96	GLY	14.5
1	B	97	LEU	14.5
1	C	59	ALA	14.4
1	C	28	ALA	14.4
1	F	16	GLY	14.3
1	B	7	VAL	14.2
1	B	23	GLY	14.1
1	B	42	THR	14.0
1	D	65	THR	13.9
1	A	23	GLY	13.9
1	A	88	CYS	13.8
1	E	4	THR	13.8
1	A	66	SER	13.6
1	C	43	GLY	13.6
1	C	49	PRO	13.5
1	E	86	VAL	13.5
1	F	70	ARG	13.4
1	A	20	LYS	13.4
1	B	103	ASN	13.3
1	C	23	GLY	13.3
1	A	110	ILE	13.2
1	E	33	TRP	13.2
1	B	61	GLY	13.2
1	D	77	LEU	13.1
1	E	13	LEU	13.1
1	C	83	TRP	13.1
1	B	29	GLY	13.1
1	E	47	SER	13.1
1	A	79	ASP	13.0
1	B	28	ALA	12.9
1	A	81	THR	12.9
1	C	3	PRO	12.9
1	D	70	ARG	12.8
1	D	34	VAL	12.8

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Mol	Chain	Res	Type	RSRZ
1	E	18	VAL	12.7
1	F	35	TYR	12.7
1	F	36	GLN	12.6
1	F	29	GLY	12.5
1	A	105	PRO	12.5
1	B	94	GLN	12.5
1	C	84	GLY	12.5
1	A	9	PRO	12.5
1	E	16	GLY	12.5
1	A	35	TYR	12.5
1	E	37	ARG	12.4
1	B	74	GLU	12.3
1	B	43	GLY	12.3
1	D	54	SER	12.2
1	E	38	ALA	12.1
1	A	32	TYR	12.1
1	D	78	PHE	12.1
1	E	61	GLY	12.0
1	C	27	GLN	12.0
1	E	72	SER	12.0
1	F	24	ALA	11.8
1	B	47	SER	11.8
1	B	34	VAL	11.8
1	E	108	VAL	11.8
1	C	85	THR	11.7
1	E	62	SER	11.7
1	D	94	GLN	11.6
1	B	111	SER	11.6
1	D	89	THR	11.6
1	F	48	ASN	11.6
1	C	13	LEU	11.6
1	C	5	ALA	11.4
1	F	73	PHE	11.4
1	F	76	PHE	11.3
1	D	56	THR	11.2
1	C	15	ASP	11.2
1	F	58	ASP	11.2
1	A	51	ASP	11.1
1	B	110	ILE	11.1
1	E	104	GLY	11.1
1	F	49	PRO	11.1
1	E	103	ASN	11.1

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Mol	Chain	Res	Type	RSRZ
1	E	88	CYS	11.0
1	D	96	GLY	11.0
1	E	6	THR	11.0
1	D	108	VAL	11.0
1	B	25	GLY	11.0
1	D	74	GLU	10.9
1	A	28	ALA	10.9
1	D	8	THR	10.9
1	A	74	GLU	10.8
1	A	64	SER	10.8
1	C	54	SER	10.7
1	C	87	ASP	10.7
1	E	56	THR	10.6
1	F	13	LEU	10.6
1	F	32	TYR	10.6
1	A	67	LEU	10.6
1	F	93	CYS	10.6
1	F	20	LYS	10.6
1	A	59	ALA	10.5
1	F	87	ASP	10.4
1	C	110	ILE	10.4
1	C	70	ARG	10.4
1	F	96	GLY	10.3
1	B	78	PHE	10.3
1	E	24	ALA	10.3
1	F	10	SER	10.3
1	F	71	ARG	10.2
1	A	83	TRP	10.1
1	C	34	VAL	10.1
1	C	71	ARG	10.1
1	D	4	THR	10.1
1	A	78	PHE	10.1
1	E	68	THR	10.0
1	E	20	LYS	10.0
1	A	99	ASP	10.0
1	F	18	VAL	10.0
1	B	112	PHE	10.0
1	C	89	THR	9.9
1	C	86	VAL	9.9
1	A	72	SER	9.9
1	C	102	GLY	9.7
1	F	47	SER	9.7

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Mol	Chain	Res	Type	RSRZ
1	A	11	SER	9.7
1	E	98	SER	9.7
1	A	36	GLN	9.7
1	A	82	ARG	9.7
1	D	6	THR	9.7
1	D	111	SER	9.6
1	C	60	ASN	9.6
1	E	10	SER	9.6
1	A	101	ALA	9.5
1	C	31	ALA	9.4
1	F	52	LEU	9.4
1	F	82	ARG	9.4
1	C	6	THR	9.4
1	E	46	ALA	9.4
1	F	112	PHE	9.3
1	A	50	ALA	9.3
1	E	27	GLN	9.2
1	B	22	ALA	9.2
1	C	80	GLY	9.2
1	B	88	CYS	9.2
1	F	94	GLN	9.2
1	B	19	VAL	9.2
1	A	44	VAL	9.2
1	A	38	ALA	9.1
1	C	82	ARG	9.0
1	E	81	THR	8.9
1	F	110	ILE	8.9
1	E	9	PRO	8.8
1	D	98	SER	8.8
1	B	63	ALA	8.8
1	E	43	GLY	8.8
1	B	101	ALA	8.8
1	F	63	ALA	8.8
1	C	108	VAL	8.8
1	F	83	TRP	8.8
1	F	103	ASN	8.7
1	E	110	ILE	8.7
1	C	52	LEU	8.7
1	C	62	SER	8.7
1	A	52	LEU	8.7
1	D	58	ASP	8.7
1	B	92	ALA	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	57	ALA	8.5
1	C	29	GLY	8.5
1	F	85	THR	8.5
1	D	42	THR	8.5
1	D	102	GLY	8.5
1	F	81	THR	8.4
1	A	30	THR	8.4
1	C	77	LEU	8.3
1	B	76	PHE	8.3
1	B	33	TRP	8.3
1	D	22	ALA	8.3
1	A	17	THR	8.3
1	C	45	HIS	8.3
1	E	28	ALA	8.3
1	B	80	GLY	8.2
1	A	7	VAL	8.2
1	B	85	THR	8.2
1	E	70	ARG	8.2
1	C	68	THR	8.2
1	F	12	GLY	8.2
1	A	10	SER	8.1
1	B	49	PRO	8.1
1	D	60	ASN	8.0
1	D	21	VAL	8.0
1	B	13	LEU	7.9
1	A	71	ARG	7.8
1	B	100	ALA	7.8
1	E	54	SER	7.8
1	D	87	ASP	7.7
1	E	35	TYR	7.7
1	C	99	ASP	7.7
1	B	36	GLN	7.6
1	E	92	ALA	7.6
1	D	35	TYR	7.6
1	A	13	LEU	7.6
1	A	95	VAL	7.6
1	B	68	THR	7.6
1	C	106	GLU	7.6
1	E	8	THR	7.5
1	F	51	ASP	7.5
1	D	61	GLY	7.5
1	F	37	ARG	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	39	ALA	7.4
1	B	75	GLY	7.4
1	D	15	ASP	7.4
1	A	54	SER	7.4
1	D	68	THR	7.3
1	A	103	ASN	7.3
1	C	66	SER	7.2
1	B	35	TYR	7.2
1	F	40	VAL	7.2
1	F	3	PRO	7.2
1	A	21	VAL	7.2
1	E	84	GLY	7.2
1	A	111	SER	7.1
1	F	45	HIS	7.1
1	E	100	ALA	7.1
1	A	97	LEU	7.0
1	B	83	TRP	7.0
1	A	87	ASP	7.0
1	B	99	ASP	6.9
1	F	80	GLY	6.9
1	C	51	ASP	6.9
1	B	69	VAL	6.9
1	D	55	VAL	6.9
1	F	33	TRP	6.9
1	E	48	ASN	6.9
1	D	105	PRO	6.8
1	B	81	THR	6.8
1	B	12	GLY	6.8
1	A	100	ALA	6.7
1	D	20	LYS	6.7
1	F	46	ALA	6.6
1	D	37	ARG	6.6
1	C	81	THR	6.5
1	B	56	THR	6.5
1	C	46	ALA	6.5
1	D	83	TRP	6.5
1	A	19	VAL	6.5
1	B	64	SER	6.5
1	D	106	GLU	6.4
1	E	40	VAL	6.4
1	C	39	ALA	6.4
1	F	39	ALA	6.4

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Mol	Chain	Res	Type	RSRZ
1	C	75	GLY	6.4
1	A	6	THR	6.4
1	B	86	VAL	6.3
1	B	87	ASP	6.3
1	C	50	ALA	6.2
1	C	113	ASN	6.2
1	D	76	PHE	6.2
1	C	103	ASN	6.2
1	B	58	ASP	6.2
1	A	33	TRP	6.2
1	F	31	ALA	6.2
1	B	79	ASP	6.2
1	A	37	ARG	6.2
1	F	72	SER	6.2
1	E	52	LEU	6.1
1	A	70	ARG	6.1
1	A	15	ASP	6.1
1	B	71	ARG	6.1
1	E	105	PRO	6.1
1	D	113	ASN	6.1
1	F	104	GLY	6.1
1	C	19	VAL	6.1
1	B	26	LEU	6.0
1	E	113	ASN	6.0
1	F	28	ALA	5.9
1	D	17	THR	5.9
1	F	17	THR	5.9
1	B	50	ALA	5.9
1	F	14	SER	5.9
1	C	58	ASP	5.9
1	A	112	PHE	5.9
1	B	67	LEU	5.9
1	B	48	ASN	5.8
1	E	73	PHE	5.8
1	F	11	SER	5.7
1	A	8	THR	5.6
1	C	112	PHE	5.6
1	B	96	GLY	5.5
1	F	92	ALA	5.5
1	C	33	TRP	5.5
1	A	27	GLN	5.5
1	E	85	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	83	TRP	5.4
1	A	49	PRO	5.4
1	E	45	HIS	5.4
1	C	4	THR	5.3
1	A	56	THR	5.3
1	F	98	SER	5.3
1	D	33	TRP	5.3
1	E	65	THR	5.2
1	B	62	SER	5.2
1	B	54	SER	5.2
1	D	80	GLY	5.1
1	A	55	VAL	5.1
1	C	11	SER	5.1
1	E	78	PHE	5.1
1	C	8	THR	5.1
1	F	68	THR	5.1
1	D	46	ALA	5.1
1	C	55	VAL	5.1
1	E	93	CYS	5.1
1	F	27	GLN	5.1
1	D	73	PHE	5.0
1	E	32	TYR	5.0
1	A	48	ASN	5.0
1	E	75	GLY	5.0
1	B	70	ARG	5.0
1	E	76	PHE	5.0
1	E	14	SER	5.0
1	E	17	THR	4.9
1	F	65	THR	4.9
1	A	107	GLY	4.9
1	F	95	VAL	4.9
1	A	4	THR	4.8
1	F	41	ASP	4.8
1	B	90	THR	4.8
1	E	50	ALA	4.7
1	D	71	ARG	4.7
1	E	94	GLN	4.7
1	B	60	ASN	4.7
1	D	7	VAL	4.7
1	A	5	ALA	4.7
1	F	69	VAL	4.6
1	A	24	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	91	ALA	4.6
1	E	74	GLU	4.6
1	A	31	ALA	4.6
1	D	63	ALA	4.6
1	B	6	THR	4.6
1	C	56	THR	4.6
1	E	42	THR	4.6
1	C	35	TYR	4.5
1	E	69	VAL	4.5
1	B	17	THR	4.5
1	A	93	CYS	4.5
1	F	15	ASP	4.5
1	C	79	ASP	4.5
1	A	77	LEU	4.5
1	D	31	ALA	4.4
1	A	25	GLY	4.4
1	D	88	CYS	4.4
1	C	37	ARG	4.4
1	B	18	VAL	4.4
1	F	74	GLU	4.4
1	E	97	LEU	4.3
1	C	95	VAL	4.3
1	C	42	THR	4.3
1	C	76	PHE	4.3
1	C	36	GLN	4.3
1	D	3	PRO	4.3
1	A	85	THR	4.3
1	E	11	SER	4.3
1	A	65	THR	4.2
1	F	66	SER	4.2
1	D	69	VAL	4.2
1	A	53	SER	4.2
1	E	106	GLU	4.2
1	B	31	ALA	4.2
1	F	61	GLY	4.1
1	A	75	GLY	4.1
1	D	107	GLY	4.1
1	A	58	ASP	4.1
1	F	86	VAL	4.1
1	C	16	GLY	4.1
1	D	67	LEU	4.1
1	E	63	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	4	THR	4.0
1	D	97	LEU	4.0
1	E	71	ARG	4.0
1	B	8	THR	4.0
1	D	36	GLN	4.0
1	E	82	ARG	4.0
1	B	52	LEU	3.9
1	C	90	THR	3.9
1	E	41	ASP	3.8
1	F	38	ALA	3.8
1	B	108	VAL	3.8
1	D	13	LEU	3.8
1	A	12	GLY	3.7
1	D	30	THR	3.7
1	F	44	VAL	3.7
1	B	45	HIS	3.7
1	D	49	PRO	3.7
1	B	82	ARG	3.7
1	B	77	LEU	3.7
1	C	105	PRO	3.6
1	D	45	HIS	3.6
1	C	107	GLY	3.6
1	E	30	THR	3.6
1	E	87	ASP	3.6
1	E	3	PRO	3.5
1	A	86	VAL	3.5
1	F	78	PHE	3.5
1	C	38	ALA	3.5
1	E	31	ALA	3.5
1	E	64	SER	3.5
1	E	66	SER	3.5
1	E	109	ALA	3.5
1	C	53	SER	3.5
1	A	34	VAL	3.4
1	A	22	ALA	3.4
1	F	106	GLU	3.4
1	D	5	ALA	3.3
1	E	102	GLY	3.3
1	B	95	VAL	3.3
1	E	55	VAL	3.3
1	F	75	GLY	3.3
1	C	98	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	78	PHE	3.2
1	F	64	SER	3.2
1	D	12	GLY	3.2
1	B	41	ASP	3.2
1	C	104	GLY	3.2
1	D	82	ARG	3.1
1	E	57	ALA	3.1
1	D	81	THR	3.1
1	C	97	LEU	3.1
1	F	77	LEU	3.0
1	C	69	VAL	3.0
1	F	26	LEU	3.0
1	B	105	PRO	3.0
1	D	9	PRO	3.0
1	B	38	ALA	3.0
1	F	30	THR	2.9
1	D	86	VAL	2.9
1	D	23	GLY	2.9
1	D	44	VAL	2.9
1	C	64	SER	2.9
1	A	47	SER	2.9
1	A	94	GLN	2.8
1	D	79	ASP	2.8
1	C	7	VAL	2.8
1	C	14	SER	2.8
1	A	42	THR	2.8
1	A	26	LEU	2.7
1	D	85	THR	2.7
1	A	40	VAL	2.7
1	E	95	VAL	2.7
1	B	2	ALA	2.7
1	C	93	CYS	2.6
1	E	12	GLY	2.6
1	B	24	ALA	2.6
1	D	43	GLY	2.6
1	F	62	SER	2.6
1	D	18	VAL	2.6
1	D	29	GLY	2.6
1	B	27	GLN	2.6
1	D	104	GLY	2.5
1	D	92	ALA	2.5
1	F	97	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	66	SER	2.5
1	F	53	SER	2.5
1	F	7	VAL	2.5
1	D	11	SER	2.4
1	A	60	ASN	2.4
1	D	66	SER	2.4
1	D	53	SER	2.4
1	E	107	GLY	2.3
1	A	18	VAL	2.3
1	D	99	ASP	2.3
1	D	62	SER	2.3
1	B	65	THR	2.3
1	C	30	THR	2.3
1	D	110	ILE	2.3
1	B	30	THR	2.3
1	C	22	ALA	2.2
1	D	57	ALA	2.2
1	D	16	GLY	2.2
1	E	23	GLY	2.2
1	B	21	VAL	2.2
1	A	76	PHE	2.2
1	B	40	VAL	2.2
1	B	98	SER	2.1
1	B	72	SER	2.1
1	A	14	SER	2.1
1	B	55	VAL	2.1
1	E	58	ASP	2.1
1	C	25	GLY	2.0

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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	F	1113	5/5	2.32	7.06	65,65,65,66	0
2	SO4	C	1114	5/5	1.70	3.67	53,53,53,54	0
3	TH2	A	1114	28/28	0.69	-0.00	27,32,58,61	0
3	TH2	F	1114	28/28	1.05	-0.03	24,31,53,54	0
2	SO4	A	1113	5/5	0.54	-0.24	77,77,78,78	0
3	TH2	C	1115	28/28	0.81	-0.28	24,29,53,53	0
3	TH2	B	1116	28/28	0.64	-0.33	12,16,45,46	0
2	SO4	E	1114	5/5	0.75	-0.37	76,76,77,77	0
3	TH2	B	1117	28/28	0.69	-0.39	28,36,53,54	0
3	TH2	E	1115	28/28	0.62	-0.53	29,34,51,52	0
3	TH2	A	1115	28/28	0.65	-0.56	58,62,84,85	0
3	TH2	D	1114	28/28	0.53	-0.83	22,34,57,59	0
2	SO4	B	1115	5/5	0.34	-1.88	41,41,42,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.