



Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 03:18 PM GMT

PDB ID : 4L2C
Title : X-ray structure of the C57R mutant of the iron superoxide dismutase from
Pseudoalteromonas haloplanktis (crystal form I)
Authors : Russo Krauss, I.; Merlino, A.; Sica, F.
Deposited on : 2013-06-04
Resolution : 1.66 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>

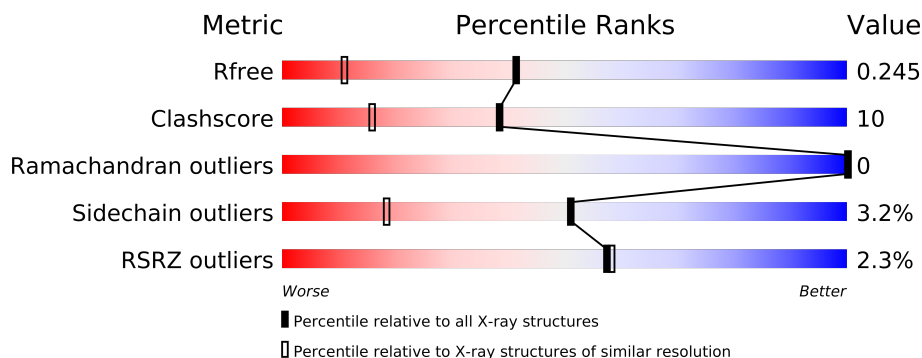
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
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) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 1.66 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}	66092	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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	192	
1	B	192	
1	C	192	
1	D	192	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	TRE	A	202	-	X
3	TRE	B	5002	-	X
3	TRE	C	202	-	X
3	TRE	D	202	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7155 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 Superoxide dismutase [Fe].

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	0	7	0
			1541	996	252	293			
1	B	192	Total	C	N	O	0	3	0
			1526	984	252	290			
1	C	192	Total	C	N	O	0	6	0
			1540	997	255	288			
1	D	192	Total	C	N	O	0	8	0
			1547	1000	256	291			

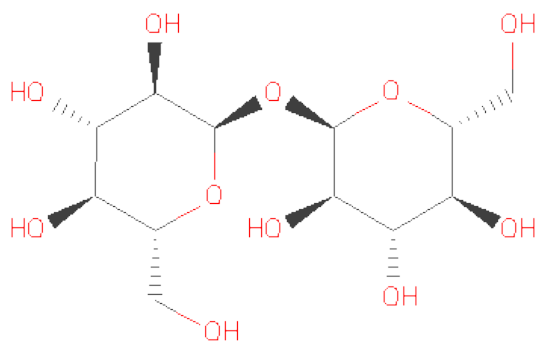
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ARG	CYS	ENGINEERED MUTATION	UNP P84612
B	57	ARG	CYS	ENGINEERED MUTATION	UNP P84612
C	57	ARG	CYS	ENGINEERED MUTATION	UNP P84612
D	57	ARG	CYS	ENGINEERED MUTATION	UNP P84612

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is TREHALOSE (three-letter code: TRE) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			23	12	11		
3	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	258	Total	O	0	1
			259	259		
4	B	248	Total	O	0	3
			251	251		
4	C	194	Total	O	0	2
			196	196		
4	D	197	Total	O	0	2
			199	199		

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.

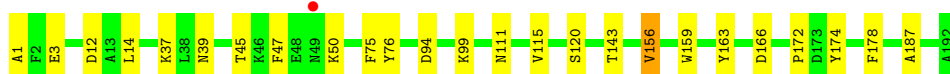
- Molecule 1: Superoxide dismutase [Fe]

Chain A: 



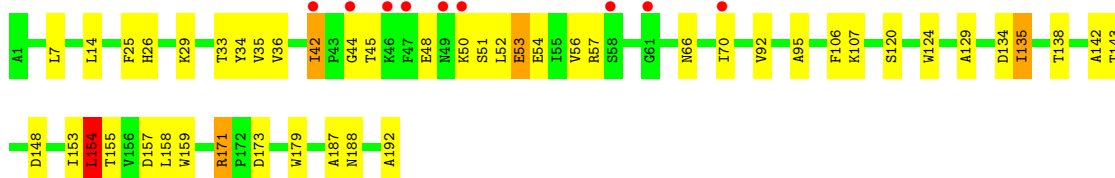
- Molecule 1: Superoxide dismutase [Fe]

Chain B: 



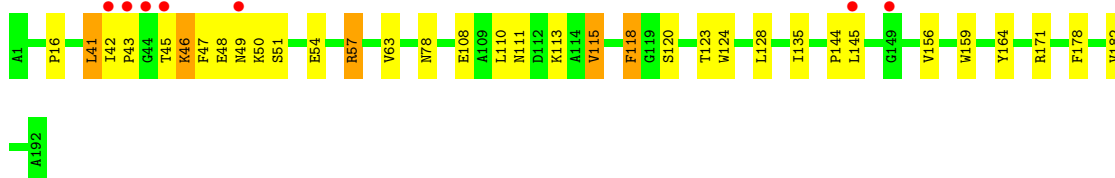
- Molecule 1: Superoxide dismutase [Fe]

Chain C: 



- Molecule 1: Superoxide dismutase [Fe]

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.49Å 103.77Å 89.83Å 90.00° 103.63° 90.00°	Depositor
Resolution (Å)	30.27 – 1.66 30.27 – 1.66	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.27-1.66) 85.5 (30.27-1.66)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.200 , 0.245 0.202 , 0.245	Depositor DCC
R_{free} test set	4570 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.9	EDS
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 95516 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7155	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 79.61 % 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 5.3722e-07. 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: TRE, FE

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	1.39	4/1618 (0.2%)	1.14	7/2215 (0.3%)
1	B	1.44	7/1587 (0.4%)	1.15	6/2170 (0.3%)
1	C	1.29	3/1613 (0.2%)	1.15	7/2205 (0.3%)
1	D	1.24	1/1628 (0.1%)	1.08	1/2225 (0.0%)
All	All	1.34	15/6446 (0.2%)	1.13	21/8815 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	TYR	CD1-CE1	7.29	1.50	1.39
1	B	76	TYR	CD1-CE1	6.98	1.49	1.39
1	A	36	VAL	CB-CG1	6.44	1.66	1.52
1	B	163	TYR	CD1-CE1	6.43	1.49	1.39
1	B	75	PHE	CE2-CZ	6.16	1.49	1.37
1	C	95	ALA	CA-CB	5.88	1.64	1.52
1	B	187	ALA	CA-CB	5.55	1.64	1.52
1	A	63	VAL	CB-CG2	5.48	1.64	1.52
1	D	118	PHE	CE2-CZ	5.36	1.47	1.37
1	A	174	TYR	CE2-CZ	5.33	1.45	1.38
1	C	129	ALA	CA-CB	5.27	1.63	1.52
1	B	156	VAL	CB-CG1	5.11	1.63	1.52
1	B	3	GLU	CG-CD	-5.09	1.44	1.51
1	C	53	GLU	CB-CG	5.05	1.61	1.52
1	A	106	PHE	CE2-CZ	5.02	1.46	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	154[A]	LEU	CA-CB-CG	7.75	133.12	115.30
1	C	154[B]	LEU	CA-CB-CG	7.75	133.12	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	ASP	CB-CG-OD1	7.73	125.25	118.30
1	A	94	ASP	CB-CG-OD1	7.67	125.21	118.30
1	C	171	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	A	76	TYR	CB-CG-CD1	6.32	124.79	121.00
1	C	171	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	D	171	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	B	14	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	B	99	LYS	CD-CE-NZ	-5.68	98.63	111.70
1	A	134	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	14	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	A	76	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	B	166	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	94	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	76	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	C	173	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	134	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	42	ILE	N-CA-C	5.25	125.18	111.00
1	A	48	GLU	C-N-CA	-5.16	108.81	121.70
1	B	12	ASP	CB-CG-OD1	5.15	122.93	118.30

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	1541	0	1452	37	0
1	B	1526	0	1435	10	0
1	C	1540	0	1463	42	0
1	D	1547	0	1466	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	23	0	22	0	0
3	B	23	0	22	0	0
3	C	23	0	22	0	0
3	D	23	0	22	1	0
4	A	259	0	0	8	0
4	B	251	0	0	4	0
4	C	196	0	0	4	0
4	D	199	0	0	5	0
All	All	7155	0	5904	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 10.

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:135:ILE:HD12	4:A:552:HOH:O	1.51	1.10
1:A:127:LYS:HB3	1:A:151[A]:THR:HG22	1.46	0.96
1:A:127:LYS:N	1:A:153[A]:ILE:HD11	1.84	0.93
1:D:42:ILE:O	1:D:45[A]:THR:HG22	1.76	0.86
1:D:43:PRO:HG2	4:D:321:HOH:O	1.76	0.84
1:A:127:LYS:HB3	1:A:151[A]:THR:CG2	2.09	0.82
1:D:111:ASN:O	1:D:115[A]:VAL:HG12	1.78	0.82
1:A:176:LYS:NZ	1:A:176:LYS:HB3	1.96	0.81
1:A:126:VAL:HA	1:A:153[A]:ILE:CD1	2.13	0.79
1:C:192:ALA:HB2	4:C:488:HOH:O	1.83	0.77
1:C:53:GLU:O	1:C:57[A]:ARG:HG3	1.85	0.76
1:A:94:ASP:HB3	4:A:327:HOH:O	1.84	0.75
1:D:51:SER:OG	1:D:54:GLU:HB2	1.88	0.74
1:D:63:VAL:HG23	4:D:304:HOH:O	1.87	0.73
1:C:153:ILE:O	1:C:154[B]:LEU:CD1	2.38	0.71
1:C:44:GLY:N	1:C:48:GLU:OE2	2.22	0.70
1:D:45[A]:THR:HG23	1:D:47:PHE:H	1.58	0.68
1:A:126:VAL:CA	1:A:153[A]:ILE:CD1	2.72	0.68
1:C:35:VAL:N	1:C:70[A]:ILE:HD11	2.07	0.68
1:C:134:ASP:C	1:C:135[A]:ILE:HD13	2.15	0.67
1:A:192:ALA:HB2	4:A:551:HOH:O	1.95	0.66
1:A:126:VAL:HA	1:A:153[A]:ILE:HD12	1.76	0.66
1:C:153:ILE:O	1:C:154[B]:LEU:HD12	1.94	0.66
1:B:156:VAL:HG22	1:B:178:PHE:CE1	2.30	0.65
1:D:45[A]:THR:HG23	1:D:47:PHE:N	2.12	0.65
1:C:35:VAL:HG22	1:C:70[A]:ILE:HD12	1.79	0.64
1:A:126:VAL:C	1:A:153[A]:ILE:CD1	2.66	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:57[A]:ARG:HH11	1:D:57[A]:ARG:HG2	1.62	0.64
1:A:57:ARG:HG2	1:A:57:ARG:HH11	1.62	0.64
1:C:52:LEU:O	1:C:56:VAL:HG23	1.98	0.64
1:D:57[A]:ARG:CG	1:D:57[A]:ARG:HH11	2.09	0.64
1:B:1:ALA:HB3	1:B:39:ASN:OD1	1.97	0.64
1:A:176:LYS:HD2	4:A:549:HOH:O	1.98	0.63
1:C:45:THR:O	1:C:48:GLU:HG3	1.99	0.62
1:D:57[A]:ARG:NH1	1:D:57[A]:ARG:HG2	2.15	0.62
1:C:53:GLU:HB3	1:C:57[B]:ARG:HH11	1.65	0.62
1:C:33:THR:HA	1:C:36[B]:VAL:HG22	1.81	0.61
1:D:78:ASN:HA	4:D:420[B]:HOH:O	1.99	0.61
1:D:46[A]:LYS:HD3	1:D:47:PHE:CE2	2.36	0.60
1:B:50:LYS:HE3	4:B:5106:HOH:O	2.01	0.60
1:A:176:LYS:CD	4:A:549:HOH:O	2.48	0.60
1:D:46[A]:LYS:HD2	4:D:443:HOH:O	2.02	0.59
1:A:92[B]:VAL:HG13	1:A:188:ASN:OD1	2.02	0.59
1:C:35:VAL:CG2	1:C:70[A]:ILE:HD12	2.32	0.59
1:A:176:LYS:HZ1	1:A:176:LYS:HB3	1.66	0.59
1:D:47:PHE:HA	1:D:50:LYS:HG2	1.86	0.58
1:C:53:GLU:HG3	4:C:366:HOH:O	2.03	0.58
1:C:138:THR:HB	1:C:142:ALA:HB3	1.85	0.58
1:A:126:VAL:CA	1:A:153[A]:ILE:HD13	2.33	0.58
1:C:34:TYR:C	1:C:70[A]:ILE:HD11	2.24	0.58
1:C:120:SER:HB3	1:C:159:TRP:CD2	2.39	0.57
1:A:126:VAL:C	1:A:153[A]:ILE:HD11	2.24	0.57
1:C:153:ILE:O	1:C:154[B]:LEU:HD13	2.03	0.56
1:A:127:LYS:N	1:A:153[A]:ILE:CD1	2.64	0.56
1:C:57[A]:ARG:NH2	1:C:148:ASP:OD1	2.40	0.55
1:C:154[A]:LEU:HD21	1:C:187:ALA:HB2	1.88	0.55
1:A:57:ARG:HG2	1:A:57:ARG:NH1	2.22	0.55
1:C:66:ASN:O	1:C:70[B]:ILE:HG13	2.06	0.55
1:B:47:PHE:HA	1:B:50:LYS:HD2	1.87	0.55
1:D:46[A]:LYS:CE	4:D:443:HOH:O	2.55	0.54
1:D:178:PHE:CZ	1:D:182[B]:VAL:HG22	2.44	0.53
1:C:51[A]:SER:OG	1:C:54:GLU:HG3	2.08	0.53
1:B:1:ALA:HB1	4:B:5329:HOH:O	2.09	0.53
1:C:134:ASP:C	1:C:135[A]:ILE:CD1	2.77	0.52
1:D:120:SER:HB3	1:D:159:TRP:CD2	2.44	0.52
1:A:176:LYS:NZ	1:A:176:LYS:CB	2.68	0.52
1:D:41[A]:LEU:HD23	1:D:63:VAL:HG22	1.92	0.52
1:B:120:SER:HB3	1:B:159:TRP:CE2	2.46	0.51
1:D:178:PHE:O	1:D:182[B]:VAL:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:92:VAL:HG22	1:C:188:ASN:OD1	2.12	0.49
1:C:33:THR:HA	1:C:36[B]:VAL:CG2	2.43	0.49
1:D:124:TRP:CE2	1:D:144:PRO:HD3	2.49	0.48
1:C:134:ASP:O	1:C:135[A]:ILE:HD12	2.13	0.48
1:A:192:ALA:CB	4:A:551:HOH:O	2.58	0.48
1:B:111:ASN:O	1:B:115[B]:VAL:HG13	2.12	0.48
1:B:120:SER:HB3	1:B:159:TRP:CD2	2.49	0.47
1:A:45:THR:O	1:A:48:GLU:HG3	2.15	0.47
1:D:42:ILE:O	1:D:45[A]:THR:CG2	2.54	0.47
1:A:120:SER:HB3	1:A:159:TRP:CD2	2.50	0.46
1:A:122:TRP:CZ3	1:A:157:ASP:HB2	2.50	0.45
1:C:26:HIS:CE1	1:C:157:ASP:OD2	2.70	0.45
1:A:53:GLU:HG3	4:A:371:HOH:O	2.15	0.45
1:A:120:SER:HB3	1:A:159:TRP:CE2	2.52	0.45
1:D:110:LEU:HA	1:D:135:ILE:HD13	1.98	0.45
1:C:50:LYS:HE3	4:C:349:HOH:O	2.17	0.44
1:D:156:VAL:HG13	1:D:156:VAL:O	2.17	0.44
1:A:126:VAL:C	1:A:153[A]:ILE:HD13	2.38	0.44
1:D:123:THR:HB	1:D:156:VAL:HG12	1.99	0.44
1:C:42:ILE:O	1:C:45:THR:HG23	2.18	0.43
1:C:154[B]:LEU:HD11	1:C:187:ALA:HB2	2.00	0.43
1:C:107:LYS:HE3	1:C:179:TRP:CG	2.53	0.43
1:C:66:ASN:O	1:C:70[A]:ILE:HG12	2.17	0.43
1:D:118:PHE:HB3	3:D:202:TRE:O6P	2.19	0.43
1:D:123:THR:HB	1:D:156:VAL:CG1	2.48	0.43
1:A:57:ARG:CG	1:A:57:ARG:HH11	2.27	0.42
1:C:120:SER:HB3	1:C:159:TRP:CE2	2.54	0.42
1:C:45:THR:HB	4:C:357:HOH:O	2.19	0.42
1:B:45:THR:HA	4:B:5124:HOH:O	2.19	0.42
1:B:37:LYS:HE3	4:B:5336:HOH:O	2.18	0.42
1:A:51:SER:OG	1:A:54:GLU:HG3	2.20	0.42
1:A:126:VAL:HA	1:A:153[A]:ILE:HD13	1.94	0.41
1:C:106:PHE:HE1	1:C:135[A]:ILE:HD11	1.85	0.41
1:C:7:LEU:HD12	1:C:7:LEU:HA	1.93	0.41
1:C:158:LEU:HD22	1:C:171:ARG:HD3	2.03	0.41
1:D:41[A]:LEU:HD23	1:D:63:VAL:CG2	2.51	0.41
1:A:124:TRP:CE3	1:A:155:THR:HB	2.56	0.41
1:C:25:PHE:O	1:C:29:LYS:HB2	2.21	0.41
1:C:124:TRP:CE3	1:C:155:THR:HB	2.56	0.40
1:A:46:LYS:HG2	4:A:304:HOH:O	2.21	0.40
1:A:176:LYS:HZ2	1:A:176:LYS:HB3	1.81	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	197/192 (103%)	192 (98%)	5 (2%)	0	100	100
1	B	193/192 (100%)	187 (97%)	6 (3%)	0	100	100
1	C	196/192 (102%)	189 (96%)	7 (4%)	0	100	100
1	D	198/192 (103%)	195 (98%)	3 (2%)	0	100	100
All	All	784/768 (102%)	763 (97%)	21 (3%)	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	165/158 (104%)	162 (98%)	3 (2%)	71	46
1	B	161/158 (102%)	159 (99%)	2 (1%)	82	63
1	C	164/158 (104%)	159 (97%)	5 (3%)	53	21
1	D	166/158 (105%)	150 (90%)	16 (10%)	12	1
All	All	656/632 (104%)	630 (96%)	26 (4%)	51	13

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	9	TYR
1	A	57	ARG
1	B	143	THR
1	B	172	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	135[A]	ILE
1	C	135[B]	ILE
1	C	143	THR
1	C	154[A]	LEU
1	C	154[B]	LEU
1	D	16	PRO
1	D	41[A]	LEU
1	D	41[B]	LEU
1	D	46[A]	LYS
1	D	46[B]	LYS
1	D	48	GLU
1	D	49	ASN
1	D	57[A]	ARG
1	D	57[B]	ARG
1	D	108	GLU
1	D	113	LYS
1	D	115[A]	VAL
1	D	115[B]	VAL
1	D	128	LEU
1	D	145	LEU
1	D	164	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	B	65	ASN
1	C	65	ASN
1	C	78	ASN

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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TRE	A	202	-	24,24,24	0.46	0	35,35,35	1.09	2 (5%)
3	TRE	B	5002	-	24,24,24	0.52	0	35,35,35	1.02	4 (11%)
3	TRE	C	202	-	24,24,24	0.45	0	35,35,35	1.24	4 (11%)
3	TRE	D	202	-	24,24,24	0.47	0	35,35,35	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRE	A	202	-	-	0/8/48/48	0/2/2/2
3	TRE	B	5002	-	-	0/8/48/48	0/2/2/2
3	TRE	C	202	-	-	0/8/48/48	0/2/2/2
3	TRE	D	202	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	202	TRE	C1P-O1-C1	-4.23	107.72	114.36
3	A	202	TRE	C1P-O1-C1	-3.77	108.43	114.36
3	C	202	TRE	O5-C5-C6	2.67	112.99	106.34
3	C	202	TRE	C6P-C5P-C4P	-2.44	107.07	113.04
3	B	5002	TRE	O5-C5-C6	2.41	112.33	106.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5002	TRE	C1P-O1-C1	-2.27	110.80	114.36
3	B	5002	TRE	C1-O5-C5	-2.21	109.45	113.73
3	A	202	TRE	O5P-C5P-C6P	2.15	111.69	106.34
3	B	5002	TRE	O5P-C5P-C6P	2.11	111.60	106.34
3	C	202	TRE	C1-O5-C5	-2.03	109.80	113.73

There are no chirality outliers.

There are no torsion outliers.

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	192/192 (100%)	-0.19	1 (0%) 88 92	7, 12, 23, 30	0
1	B	192/192 (100%)	-0.21	1 (0%) 88 92	7, 12, 20, 30	0
1	C	192/192 (100%)	0.27	9 (4%) 30 28	11, 17, 29, 41	0
1	D	192/192 (100%)	0.18	7 (3%) 41 41	11, 17, 30, 43	0
All	All	768/768 (100%)	0.01	18 (2%) 57 58	7, 15, 27, 43	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	49	ASN	4.4
1	D	49	ASN	4.3
1	C	47	PHE	3.6
1	C	46	LYS	3.3
1	C	58	SER	3.2
1	D	44	GLY	3.1
1	D	42	ILE	3.0
1	C	44	GLY	2.8
1	C	50	LYS	2.6
1	A	49	ASN	2.6
1	C	42	ILE	2.6
1	D	149	GLY	2.5
1	B	49	ASN	2.4
1	D	45[A]	THR	2.4
1	D	145	LEU	2.3
1	C	61	GLY	2.3
1	C	70[A]	ILE	2.2
1	D	43	PRO	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 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
3	TRE	A	202	23/23	0.19	8.67	16,24,29,31	0
3	TRE	B	5002	23/23	0.14	5.60	17,23,30,32	0
3	TRE	D	202	23/23	0.22	3.60	28,33,38,40	0
3	TRE	C	202	23/23	0.17	2.97	21,27,36,39	0
2	FE	B	5001	1/1	0.07	-3.22	9,9,9,9	0
2	FE	A	201	1/1	0.05	-3.47	9,9,9,9	0
2	FE	D	201	1/1	0.08	-4.07	13,13,13,13	0
2	FE	C	201	1/1	0.06	-5.41	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.