



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:41 am BST

PDB ID : 2V41
Title : Crystal Structure of the C45S mutant of the Peroxiredoxin 6 of Arenicola Marina. Orthorhombic form
Authors : Smeets, A.; Declercq, J.P.
Deposited on : 2007-06-27
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

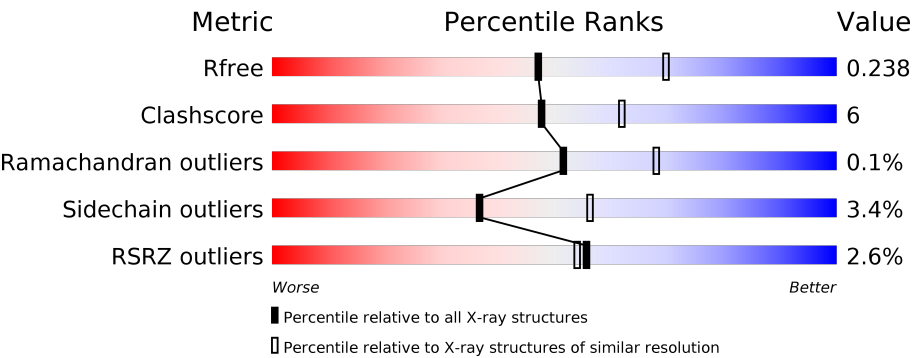
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	233	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>79%14%• 6%</div></div>
1	B	233	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>84%11%6%</div></div>
1	C	233	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>80%12%7%</div></div>
1	D	233	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>81%13%6%</div></div>
1	E	233	<div><div>5%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>74%19%• 6%</div></div>
1	F	233	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>82%12%• 6%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	233	<div><div></div><div>4%</div><div>78%</div><div>16%</div><div>6%</div></div>
1	H	233	<div><div></div><div>3%</div><div>80%</div><div>12%</div><div>6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13959 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 PEROXIREDOXIN 6..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1703	1087	288	319	9			
1	B	220	Total	C	N	O	S	0	0	0
			1703	1087	288	319	9			
1	C	216	Total	C	N	O	S	0	0	0
			1672	1068	282	313	9			
1	D	220	Total	C	N	O	S	0	0	0
			1703	1087	288	319	9			
1	E	220	Total	C	N	O	S	0	0	0
			1703	1087	288	319	9			
1	F	220	Total	C	N	O	S	0	0	0
			1703	1087	288	319	9			
1	G	220	Total	C	N	O	S	0	0	0
			1703	1087	288	319	9			
1	H	220	Total	C	N	O	S	0	0	0
			1703	1087	288	319	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	SER	CYS	engineered mutation	UNP Q1AN22
B	45	SER	CYS	engineered mutation	UNP Q1AN22
C	45	SER	CYS	engineered mutation	UNP Q1AN22
D	45	SER	CYS	engineered mutation	UNP Q1AN22
E	45	SER	CYS	engineered mutation	UNP Q1AN22
F	45	SER	CYS	engineered mutation	UNP Q1AN22
G	45	SER	CYS	engineered mutation	UNP Q1AN22
H	45	SER	CYS	engineered mutation	UNP Q1AN22

- Molecule 2 is BENZOIC ACID (three-letter code: BEZ) (formula: C₇H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	7	2		
2	B	1	Total	C	O	0	0
			9	7	2		
2	C	1	Total	C	O	0	0
			9	7	2		
2	D	1	Total	C	O	0	0
			9	7	2		
2	E	1	Total	C	O	0	0
			9	7	2		
2	F	1	Total	C	O	0	0
			9	7	2		
2	G	1	Total	C	O	0	0
			9	7	2		
2	H	1	Total	C	O	0	0
			9	7	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	48	Total	O	0	0
			48	48		
3	C	33	Total	O	0	0
			33	33		
3	D	39	Total	O	0	0
			39	39		

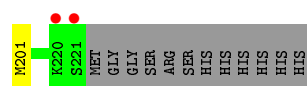
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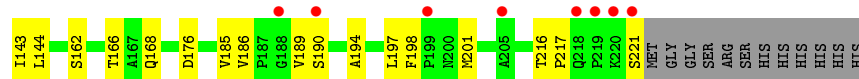
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	31	Total 31	O 31	0	0
3	F	30	Total 30	O 30	0	0
3	G	33	Total 33	O 33	0	0
3	H	34	Total 34	O 34	0	0

- Molecule 1: PEROXIREDOXIN 6.

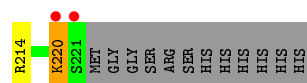
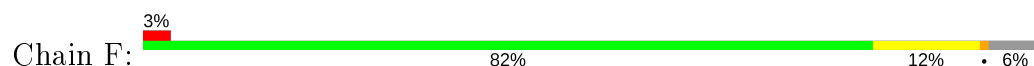




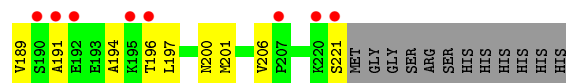
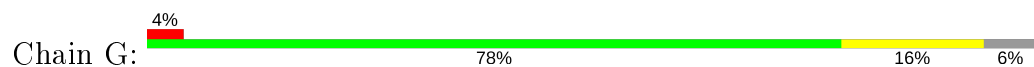
- Molecule 1: PEROXIREDOXIN 6.



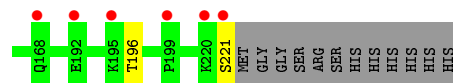
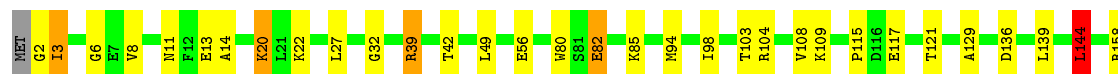
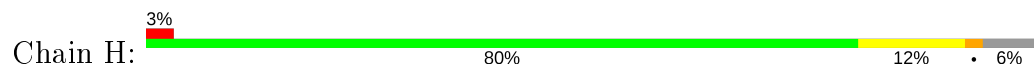
- Molecule 1: PEROXIREDOXIN 6.



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- Molecule 1: PEROXIREDOXIN 6.



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.11Å 111.16Å 229.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.40) 97.8 (15.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.239 0.180 , 0.238	Depositor DCC
R_{free} test set	3823 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13959	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: BEZ

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	0.92	0/1742	0.90	1/2362 (0.0%)
1	B	0.93	1/1742 (0.1%)	0.92	7/2362 (0.3%)
1	C	0.91	0/1710	0.88	5/2319 (0.2%)
1	D	0.84	0/1742	0.87	2/2362 (0.1%)
1	E	0.85	1/1742 (0.1%)	0.89	4/2362 (0.2%)
1	F	0.82	0/1742	0.82	1/2362 (0.0%)
1	G	0.82	0/1742	0.86	0/2362
1	H	0.88	2/1742 (0.1%)	0.88	4/2362 (0.2%)
All	All	0.87	4/13904 (0.0%)	0.88	24/18853 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	82	GLU	CD-OE1	8.30	1.34	1.25
1	E	79	GLU	CD-OE1	7.74	1.34	1.25
1	H	82	GLU	CD-OE2	6.79	1.33	1.25
1	B	183	CYS	CB-SG	-6.63	1.71	1.82

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	ASP	CB-CG-OD1	8.36	125.82	118.30
1	H	158	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	158	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	181	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	C	182	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	E	79	GLU	OE1-CD-OE2	6.50	131.09	123.30
1	A	182	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	E	176	ASP	CB-CG-OD1	6.34	124.01	118.30
1	C	62	ARG	NE-CZ-NH1	6.14	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	144	LEU	CB-CG-CD1	5.82	120.89	111.00
1	B	62	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	H	136	ASP	CB-CG-OD1	5.68	123.41	118.30
1	E	118	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	E	62	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	C	58	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	H	39	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	D	39	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	25	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	62	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	144	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	C	62	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	C	182	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	158	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	F	158	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1703	0	1723	28	0
1	B	1703	0	1723	14	0
1	C	1672	0	1690	30	0
1	D	1703	0	1723	21	0
1	E	1703	0	1723	35	0
1	F	1703	0	1723	19	0
1	G	1703	0	1723	27	0
1	H	1703	0	1723	18	0
2	A	9	0	5	0	0
2	B	9	0	5	0	0
2	C	9	0	5	1	0
2	D	9	0	5	0	0
2	E	9	0	5	0	0
2	F	9	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	9	0	5	0	0
2	H	9	0	5	1	0
3	A	46	0	0	0	0
3	B	48	0	0	0	0
3	C	33	0	0	1	0
3	D	39	0	0	1	0
3	E	31	0	0	1	0
3	F	30	0	0	1	0
3	G	33	0	0	0	0
3	H	34	0	0	1	0
All	All	13959	0	13791	168	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 6.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:VAL:HG21	1:B:201:MET:HE2	1.17	1.16
1:C:34:LEU:HD12	1:C:67:ILE:HG23	1.23	1.11
1:C:216:THR:HG21	1:G:121:THR:HG22	1.45	0.98
1:D:185:VAL:HG21	1:D:201:MET:CE	1.94	0.96
1:D:185:VAL:HG21	1:D:201:MET:HE2	1.50	0.94
1:A:185:VAL:HG21	1:A:201:MET:CE	1.97	0.93
1:E:185:VAL:HG21	1:E:201:MET:HE2	1.54	0.87
1:A:185:VAL:HG21	1:A:201:MET:HE2	1.55	0.87
1:D:34:LEU:HD13	1:D:67:ILE:HG23	1.61	0.82
1:A:171:VAL:HG11	1:A:219:PRO:HG2	1.66	0.78
1:G:185:VAL:HG21	1:G:201:MET:HE2	1.64	0.77
1:E:57:GLY:O	1:E:61:LYS:HG2	1.85	0.77
1:C:216:THR:CG2	1:G:121:THR:HG22	2.16	0.76
1:C:34:LEU:CD1	1:C:67:ILE:HG23	2.11	0.76
1:C:34:LEU:HD12	1:C:67:ILE:CG2	2.13	0.74
1:C:183:CYS:H	1:C:216:THR:HG22	1.53	0.73
1:E:3:ILE:HG12	1:E:139:LEU:HD22	1.71	0.71
1:C:185:VAL:HG11	1:C:201:MET:CE	2.20	0.71
1:A:185:VAL:HG21	1:A:201:MET:HE3	1.75	0.69
1:A:40:ASP:OD2	1:A:77:HIS:HD2	1.77	0.68
1:A:60:LYS:HD3	1:H:108:VAL:HG13	1.76	0.67
1:H:3:ILE:HG12	1:H:139:LEU:HD22	1.77	0.67
1:D:40:ASP:OD2	1:D:77:HIS:CD2	2.48	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:VAL:HG21	1:E:201:MET:CE	2.25	0.66
1:C:108:VAL:CG1	1:E:61:LYS:HD2	2.26	0.66
1:B:40:ASP:OD2	1:B:77:HIS:HD2	1.78	0.66
1:E:162:SER:O	1:E:166:THR:HG23	1.96	0.66
1:C:60:LYS:HG2	1:H:8:VAL:HB	1.79	0.65
1:E:49:LEU:HD13	1:E:80:TRP:HH2	1.63	0.63
1:E:194:ALA:HB1	1:E:201:MET:HE3	1.80	0.62
1:C:40:ASP:OD2	1:C:77:HIS:HD2	1.82	0.61
1:E:67:ILE:HD12	1:E:97:PRO:HG2	1.83	0.61
1:D:143:ILE:HD12	1:D:145:TYR:CE1	2.36	0.60
1:D:67:ILE:HG12	1:D:99:ILE:HD12	1.83	0.60
1:A:185:VAL:CG2	1:A:201:MET:HE2	2.31	0.60
1:C:182:ARG:NH2	3:C:2032:HOH:O	2.35	0.60
1:E:168:GLN:HG3	1:E:221:SER:HB2	1.84	0.60
1:B:77:HIS:CE1	1:B:98:ILE:HG22	2.36	0.60
1:C:183:CYS:H	1:C:216:THR:CG2	2.13	0.60
1:E:48:GLU:O	1:E:52:VAL:HG23	2.02	0.60
1:E:40:ASP:OD2	1:E:77:HIS:HD2	1.85	0.60
1:G:40:ASP:OD2	1:G:77:HIS:HD2	1.85	0.60
1:D:109:LYS:NZ	3:D:2024:HOH:O	2.35	0.60
1:E:119:THR:HG22	1:E:125:LEU:HD21	1.83	0.59
1:D:40:ASP:OD2	1:D:77:HIS:HD2	1.84	0.59
1:D:166:THR:HG22	1:D:171:VAL:O	2.03	0.58
1:E:194:ALA:HB1	1:E:201:MET:CE	2.33	0.58
1:E:185:VAL:HG11	1:E:201:MET:HE1	1.86	0.58
1:F:121:THR:CG2	1:F:123:MET:HG3	2.33	0.58
1:C:108:VAL:HG13	1:E:61:LYS:HD2	1.86	0.57
1:E:57:GLY:O	1:E:61:LYS:CG	2.53	0.56
1:E:77:HIS:CE1	1:E:98:ILE:HG22	2.41	0.56
1:E:59:PHE:CB	1:E:66:LEU:HD11	2.36	0.56
1:G:34:LEU:HD13	1:G:67:ILE:HG23	1.87	0.56
1:A:64:VAL:HG21	1:A:160:ILE:HD13	1.88	0.55
1:F:121:THR:HG22	3:F:2015:HOH:O	2.08	0.54
1:E:86:CYS:SG	1:F:207:PRO:HD3	2.48	0.53
1:G:29:ASN:CG	1:G:29:ASN:O	2.46	0.53
1:E:43:PRO:HG3	1:F:212:TYR:O	2.09	0.53
1:E:59:PHE:CG	1:E:66:LEU:HD11	2.42	0.53
1:C:168:GLN:HE22	1:G:118:ARG:NE	2.07	0.52
1:C:204:LYS:HB3	1:C:213:LEU:HD23	1.92	0.52
1:D:11:ASN:CG	1:D:22:LYS:NZ	2.64	0.51
1:H:82:GLU:OE2	1:H:85:LYS:NZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:LEU:HD12	1:G:21:LEU:O	2.10	0.51
1:E:190:SER:HA	3:E:2026:HOH:O	2.09	0.51
1:C:216:THR:CG2	1:G:121:THR:CG2	2.87	0.51
1:C:216:THR:HG21	1:G:121:THR:CG2	2.32	0.51
1:A:174:PRO:HA	1:B:44:VAL:HG13	1.93	0.50
1:A:217:PRO:O	1:A:218:GLN:C	2.49	0.50
1:E:186:VAL:CG2	1:E:189:VAL:HG23	2.41	0.50
1:B:185:VAL:HG21	1:B:201:MET:CE	2.12	0.50
1:B:185:VAL:CG2	1:B:201:MET:HE2	2.12	0.50
1:F:27:LEU:HD11	1:F:32:GLY:HA3	1.93	0.50
1:E:49:LEU:HD13	1:E:80:TRP:CH2	2.43	0.50
1:C:117:GLU:CD	2:C:1218:BEZ:H4	2.32	0.49
1:H:2:GLY:N	3:H:2001:HOH:O	2.45	0.49
1:C:44:VAL:HG13	1:D:174:PRO:HA	1.93	0.49
1:H:117:GLU:HA	1:H:117:GLU:OE1	2.13	0.49
1:B:119:THR:OG1	1:B:123:MET:HB2	2.13	0.49
1:D:34:LEU:HD13	1:D:67:ILE:CG2	2.39	0.49
1:A:81:SER:O	1:A:85:LYS:HG3	2.13	0.49
1:F:117:GLU:CD	2:F:1222:BEZ:H4	2.33	0.48
1:H:11:ASN:O	1:H:22:LYS:HE2	2.12	0.48
1:F:121:THR:HG23	1:F:123:MET:HG3	1.93	0.48
1:B:185:VAL:HG11	1:B:201:MET:HE1	1.96	0.48
1:A:189:VAL:HG12	1:A:194:ALA:HB2	1.95	0.48
1:C:115:PRO:HB3	1:D:6:GLY:HA3	1.95	0.48
1:A:219:PRO:O	1:A:220:LYS:C	2.51	0.48
1:C:40:ASP:OD2	1:C:77:HIS:CD2	2.64	0.47
1:A:3:ILE:HD13	1:A:9:PHE:CD1	2.49	0.47
1:A:168:GLN:CG	1:H:121:THR:HG21	2.44	0.47
1:C:108:VAL:CG1	1:E:61:LYS:CD	2.93	0.47
1:G:153:PHE:CD1	1:G:156:ILE:HD12	2.50	0.47
1:D:112:MET:O	1:D:126:THR:HA	2.15	0.47
1:G:196:THR:HG22	1:G:197:LEU:HD12	1.97	0.46
1:G:115:PRO:HB3	1:H:6:GLY:HA3	1.96	0.46
1:F:49:LEU:HB3	1:F:84:VAL:HG11	1.96	0.46
1:D:27:LEU:HD11	1:D:32:GLY:HA3	1.96	0.46
1:E:57:GLY:O	1:E:61:LYS:CD	2.64	0.46
1:C:3:ILE:HG12	1:C:139:LEU:HD22	1.98	0.46
1:F:203:VAL:HG22	1:F:214:ARG:HG2	1.97	0.46
1:A:13:GLU:HG2	1:A:22:LYS:HD2	1.98	0.46
1:A:13:GLU:HA	1:A:21:LEU:O	2.17	0.45
1:A:47:THR:HG22	1:A:87:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:HIS:HE1	1:B:99:ILE:O	1.99	0.45
1:F:55:LEU:O	1:F:58:ASP:HB2	2.17	0.45
1:B:21:LEU:HD12	1:B:21:LEU:O	2.16	0.45
1:F:119:THR:OG1	1:F:121:THR:HG22	2.17	0.45
1:H:94:MET:CE	1:H:98:ILE:HD11	2.47	0.45
1:F:10:PRO:HB3	1:F:109:LYS:HE2	1.98	0.45
1:F:121:THR:HG21	1:F:123:MET:HG3	1.99	0.45
1:G:173:THR:HB	1:G:177:TRP:CG	2.51	0.45
1:C:14:ALA:HB1	1:C:99:ILE:HG23	1.99	0.45
1:A:48:GLU:O	1:A:52:VAL:HG23	2.18	0.44
1:D:67:ILE:HG12	1:D:99:ILE:CD1	2.47	0.44
1:B:194:ALA:HB1	1:B:201:MET:CE	2.47	0.44
1:A:153:PHE:HA	1:A:156:ILE:HD12	1.99	0.44
1:G:27:LEU:HD11	1:G:32:GLY:HA3	1.99	0.44
1:C:34:LEU:HD11	1:C:99:ILE:HD12	2.00	0.44
1:G:21:LEU:HD12	1:G:21:LEU:C	2.37	0.44
1:G:119:THR:OG1	1:G:123:MET:HB2	2.17	0.44
1:G:3:ILE:HG12	1:G:139:LEU:HD22	1.99	0.44
1:C:162:SER:O	1:C:166:THR:HG23	2.18	0.43
1:G:191:ALA:O	1:G:194:ALA:HB3	2.18	0.43
1:G:6:GLY:HA3	1:H:115:PRO:HB3	1.99	0.43
1:E:6:GLY:HA3	1:F:115:PRO:HB3	2.00	0.43
1:F:68:ALA:HB3	1:F:98:ILE:HG12	2.00	0.43
1:C:168:GLN:NE2	1:G:118:ARG:NE	2.66	0.43
1:B:198:PHE:HB2	1:B:201:MET:HE3	2.01	0.43
1:H:27:LEU:HD11	1:H:32:GLY:HA3	1.99	0.43
1:F:121:THR:HG23	1:F:123:MET:CG	2.49	0.43
1:A:47:THR:HA	1:A:87:LEU:CD1	2.48	0.43
1:D:26:TRP:CH2	1:D:67:ILE:HB	2.54	0.42
1:E:59:PHE:HB2	1:E:66:LEU:HD11	2.00	0.42
1:G:29:ASN:OD1	1:G:29:ASN:O	2.36	0.42
1:H:49:LEU:HD13	1:H:80:TRP:HH2	1.84	0.42
1:A:201:MET:HE1	1:A:214:ARG:HD2	2.00	0.42
1:D:153:PHE:HA	1:D:156:ILE:HD12	2.02	0.42
1:H:42:THR:HB	2:H:1222:BEZ:C	2.50	0.42
1:A:57:GLY:O	1:A:61:LYS:HG3	2.20	0.42
1:D:11:ASN:CG	1:D:22:LYS:HZ3	2.23	0.42
1:D:52:VAL:CG1	1:D:66:LEU:HD13	2.50	0.42
1:E:14:ALA:HB1	1:E:99:ILE:HG23	2.02	0.42
1:A:220:LYS:HD2	1:A:220:LYS:HA	1.95	0.42
1:G:200:ASN:HD22	1:G:200:ASN:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLN:HG3	1:H:121:THR:HG21	2.00	0.42
1:D:185:VAL:CG2	1:D:201:MET:CE	2.82	0.42
1:F:220:LYS:NZ	1:F:220:LYS:O	2.33	0.41
1:E:216:THR:HG23	1:E:217:PRO:O	2.20	0.41
1:G:194:ALA:HB1	1:G:201:MET:HE3	2.03	0.41
1:C:108:VAL:HG11	1:E:61:LYS:HG3	2.02	0.41
1:B:48:GLU:O	1:B:52:VAL:HG23	2.21	0.41
1:C:174:PRO:HG2	1:C:182:ARG:NH2	2.36	0.41
1:G:44:VAL:O	1:G:48:GLU:HG3	2.20	0.41
1:H:103:THR:O	1:H:104:ARG:HB2	2.20	0.41
1:A:182:ARG:HB3	1:A:217:PRO:HA	2.03	0.41
1:A:6:GLY:HA3	1:B:115:PRO:HB3	2.03	0.41
1:C:108:VAL:HG11	1:E:61:LYS:CD	2.51	0.40
1:A:26:TRP:CH2	1:A:65:LYS:HB3	2.56	0.40
1:E:197:LEU:HD23	1:E:198:PHE:CE2	2.56	0.40
1:F:49:LEU:O	1:F:96:TYR:OH	2.38	0.40
1:G:186:VAL:O	1:G:189:VAL:HG12	2.21	0.40
1:G:48:GLU:O	1:G:52:VAL:HG23	2.22	0.40
1:H:14:ALA:O	1:H:20:LYS:HA	2.21	0.40
1:E:36:SER:HA	1:E:69:LEU:O	2.21	0.40
1:F:40:ASP:OD2	1:F:77:HIS:CD2	2.74	0.40
1:H:129:ALA:HB2	1:H:144:LEU:HD12	2.03	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	218/233 (94%)	209 (96%)	9 (4%)	0	100	100
1	B	218/233 (94%)	211 (97%)	7 (3%)	0	100	100
1	C	214/233 (92%)	205 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	218/233 (94%)	213 (98%)	5 (2%)	0	100	100
1	E	218/233 (94%)	211 (97%)	6 (3%)	1 (0%)	29	41
1	F	218/233 (94%)	212 (97%)	6 (3%)	0	100	100
1	G	218/233 (94%)	206 (94%)	12 (6%)	0	100	100
1	H	218/233 (94%)	210 (96%)	8 (4%)	0	100	100
All	All	1740/1864 (93%)	1677 (96%)	62 (4%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	43	PRO

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	189/200 (94%)	185 (98%)	4 (2%)	53	72
1	B	189/200 (94%)	185 (98%)	4 (2%)	53	72
1	C	185/200 (92%)	179 (97%)	6 (3%)	39	59
1	D	189/200 (94%)	183 (97%)	6 (3%)	39	59
1	E	189/200 (94%)	180 (95%)	9 (5%)	25	41
1	F	189/200 (94%)	182 (96%)	7 (4%)	34	53
1	G	189/200 (94%)	182 (96%)	7 (4%)	34	53
1	H	189/200 (94%)	180 (95%)	9 (5%)	25	41
All	All	1508/1600 (94%)	1456 (97%)	52 (3%)	37	56

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	21	LEU

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Mol	Chain	Res	Type
1	A	87	LEU
1	A	144	LEU
1	B	22	LYS
1	B	87	LEU
1	B	118	ARG
1	B	195	LYS
1	C	87	LEU
1	C	123	MET
1	C	143	ILE
1	C	182	ARG
1	C	206	VAL
1	C	216	THR
1	D	39	ARG
1	D	61	LYS
1	D	82	GLU
1	D	144	LEU
1	D	196	THR
1	D	197	LEU
1	E	3	ILE
1	E	30	SER
1	E	49	LEU
1	E	56	GLU
1	E	72	ASP
1	E	86	CYS
1	E	87	LEU
1	E	143	ILE
1	E	144	LEU
1	F	29	ASN
1	F	87	LEU
1	F	123	MET
1	F	143	ILE
1	F	168	GLN
1	F	202	GLU
1	F	220	LYS
1	G	29	ASN
1	G	56	GLU
1	G	60	LYS
1	G	87	LEU
1	G	143	ILE
1	G	206	VAL
1	G	221	SER
1	H	3	ILE

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Mol	Chain	Res	Type
1	H	13	GLU
1	H	20	LYS
1	H	39	ARG
1	H	56	GLU
1	H	109	LYS
1	H	144	LEU
1	H	196	THR
1	H	221	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	77	HIS
1	C	77	HIS
1	C	168	GLN
1	C	178	GLN
1	D	77	HIS
1	D	178	GLN
1	E	77	HIS
1	E	178	GLN
1	F	178	GLN
1	G	77	HIS
1	G	178	GLN
1	G	200	ASN
1	H	77	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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

8 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	BEZ	C	1218	-	7,9,9	1.42	1 (14%)	8,11,11	0.89	0
2	BEZ	A	1222	-	7,9,9	0.60	0	8,11,11	1.44	2 (25%)
2	BEZ	B	1222	-	7,9,9	1.43	1 (14%)	8,11,11	1.28	1 (12%)
2	BEZ	D	1222	-	7,9,9	1.47	1 (14%)	8,11,11	1.01	0
2	BEZ	E	1222	-	7,9,9	0.91	0	8,11,11	1.58	2 (25%)
2	BEZ	F	1222	-	7,9,9	1.48	1 (14%)	8,11,11	1.58	2 (25%)
2	BEZ	G	1222	-	7,9,9	1.10	1 (14%)	8,11,11	1.21	1 (12%)
2	BEZ	H	1222	-	7,9,9	0.46	0	8,11,11	1.27	1 (12%)

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	BEZ	C	1218	-	-	0/0/4/4	0/1/1/1
2	BEZ	A	1222	-	-	0/0/4/4	0/1/1/1
2	BEZ	B	1222	-	-	0/0/4/4	0/1/1/1
2	BEZ	D	1222	-	-	0/0/4/4	0/1/1/1
2	BEZ	E	1222	-	-	0/0/4/4	0/1/1/1
2	BEZ	F	1222	-	-	0/0/4/4	0/1/1/1
2	BEZ	G	1222	-	-	0/0/4/4	0/1/1/1
2	BEZ	H	1222	-	-	0/0/4/4	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1222	BEZ	C1-C	3.50	1.50	1.47
2	B	1222	BEZ	C1-C	3.48	1.50	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1222	BEZ	C1-C	3.38	1.50	1.47
2	C	1218	BEZ	C1-C	3.34	1.50	1.47
2	G	1222	BEZ	C1-C	2.79	1.50	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1222	BEZ	C6-C1-C	-2.65	116.81	120.37
2	A	1222	BEZ	C3-C2-C1	-2.58	117.32	120.56
2	F	1222	BEZ	C3-C2-C1	-2.56	117.34	120.56
2	E	1222	BEZ	C6-C1-C2	2.52	122.61	117.59
2	A	1222	BEZ	C6-C1-C2	2.37	122.30	117.59
2	F	1222	BEZ	C6-C1-C2	2.30	122.17	117.59
2	B	1222	BEZ	C4-C3-C2	-2.24	116.77	120.19
2	H	1222	BEZ	C5-C6-C1	-2.19	117.80	120.56
2	G	1222	BEZ	C4-C3-C2	-2.01	117.13	120.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1218	BEZ	1	0
2	F	1222	BEZ	1	0
2	H	1222	BEZ	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	220/233 (94%)	-0.36	2 (0%) 84 82	34, 40, 46, 62	0
1	B	220/233 (94%)	-0.33	4 (1%) 68 66	33, 40, 47, 58	0
1	C	216/233 (92%)	-0.35	5 (2%) 60 58	34, 41, 45, 50	0
1	D	220/233 (94%)	-0.26	3 (1%) 75 73	34, 40, 47, 58	0
1	E	220/233 (94%)	-0.03	11 (5%) 28 27	34, 41, 47, 53	0
1	F	220/233 (94%)	-0.09	6 (2%) 54 52	35, 41, 47, 51	0
1	G	220/233 (94%)	-0.16	9 (4%) 37 36	35, 41, 47, 49	0
1	H	220/233 (94%)	-0.19	6 (2%) 54 52	35, 40, 46, 52	0
All	All	1756/1864 (94%)	-0.22	46 (2%) 56 54	33, 41, 47, 62	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	221	SER	6.6
1	H	221	SER	6.0
1	A	221	SER	5.5
1	G	221	SER	5.1
1	B	221	SER	3.9
1	F	191	ALA	3.9
1	D	188	GLY	3.7
1	E	220	LYS	3.6
1	G	191	ALA	3.5
1	G	196	THR	3.4
1	G	190	SER	3.3
1	F	221	SER	3.2
1	H	192	GLU	3.2
1	H	220	LYS	3.1
1	F	220	LYS	3.0
1	E	190	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	188	GLY	2.9
1	F	93	ASP	2.9
1	G	195	LYS	2.9
1	D	220	LYS	2.8
1	A	220	LYS	2.8
1	E	92	GLY	2.8
1	E	84	VAL	2.8
1	G	192	GLU	2.8
1	E	221	SER	2.8
1	E	91	LYS	2.7
1	B	92	GLY	2.6
1	C	185	VAL	2.6
1	G	207	PRO	2.6
1	F	120	SER	2.6
1	E	219	PRO	2.5
1	G	220	LYS	2.5
1	E	199	PRO	2.4
1	G	168	GLN	2.4
1	E	205	ALA	2.4
1	C	92	GLY	2.3
1	E	218	GLN	2.3
1	F	29	ASN	2.2
1	C	182	ARG	2.1
1	H	168	GLN	2.1
1	C	200	ASN	2.1
1	C	199	PRO	2.0
1	H	199	PRO	2.0
1	B	120	SER	2.0
1	B	122	GLY	2.0
1	H	195	LYS	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BEZ	E	1222	9/9	0.94	0.22	42,42,43,43	0
2	BEZ	F	1222	9/9	0.95	0.24	47,48,49,49	0
2	BEZ	H	1222	9/9	0.96	0.21	39,39,40,40	0
2	BEZ	D	1222	9/9	0.97	0.19	31,33,35,36	0
2	BEZ	C	1218	9/9	0.97	0.23	36,37,38,38	0
2	BEZ	A	1222	9/9	0.98	0.18	25,28,29,29	0
2	BEZ	G	1222	9/9	0.98	0.18	30,33,33,34	0
2	BEZ	B	1222	9/9	0.98	0.19	29,30,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.