



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 06:56 PM EDT

PDB ID : 2R9P / pdb_00002r9p
Title : Human mesotrypsin complexed with bovine pancreatic trypsin inhibitor(BPTI)
Authors : Salameh, M.A.; Soares, A.S.; Radisky, E.S.
Deposited on : 2007-09-13
Resolution : 1.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

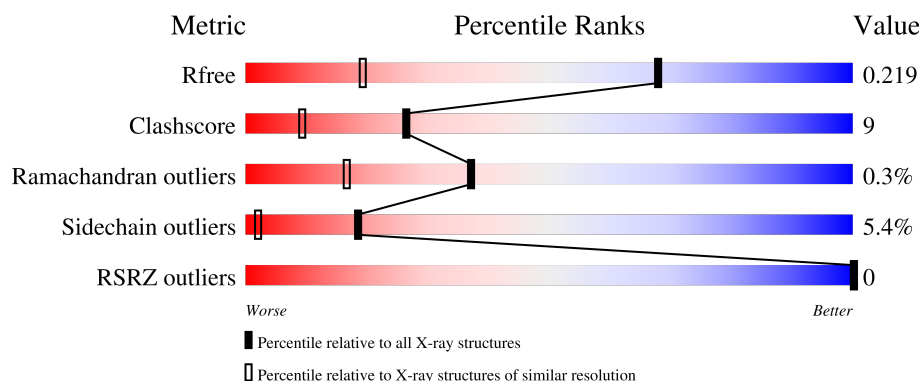
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 1.40 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}	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	224	 80% 18% .
1	B	224	 80% 16% .
1	C	224	 81% 18% .
1	D	224	 77% 21% .
2	E	58	 84% 12% .

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Mol	Chain	Length	Quality of chain
2	F	58	
2	G	58	
2	I	58	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	14	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9414 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 Trypsin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	12	2	0
			1713	1080	296	325	12			
1	B	224	Total	C	N	O	S	16	3	0
			1717	1080	297	328	12			
1	C	224	Total	C	N	O	S	11	1	0
			1708	1075	296	325	12			
1	D	224	Total	C	N	O	S	15	2	0
			1711	1077	296	326	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	SER	engineered mutation	UNP P35030
B	195	ALA	SER	engineered mutation	UNP P35030
C	195	ALA	SER	engineered mutation	UNP P35030
D	195	ALA	SER	engineered mutation	UNP P35030

- Molecule 2 is a protein called Pancreatic trypsin inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	58	Total	C	N	O	S	8	0	0
			454	284	84	79	7			
2	E	58	Total	C	N	O	S	3	0	0
			454	284	84	79	7			
2	F	58	Total	C	N	O	S	13	0	0
			454	284	84	79	7			
2	G	58	Total	C	N	O	S	16	0	0
			454	284	84	79	7			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	1
			10	8	2		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

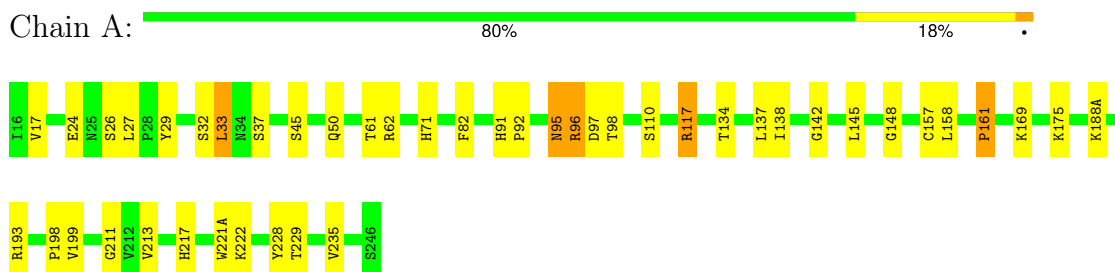
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	3
			176	176		
4	B	128	Total	O	0	1
			129	129		
4	C	98	Total	O	0	4
			102	102		
4	D	101	Total	O	0	0
			101	101		
4	I	29	Total	O	0	1
			30	30		
4	E	41	Total	O	0	0
			41	41		
4	F	30	Total	O	0	1
			31	31		
4	G	33	Total	O	0	1
			34	34		

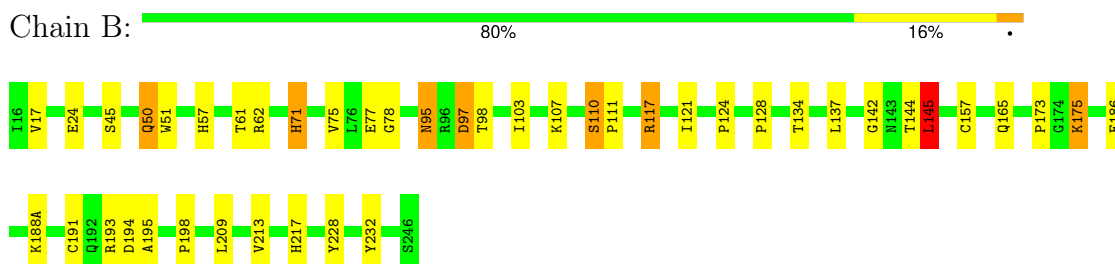
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

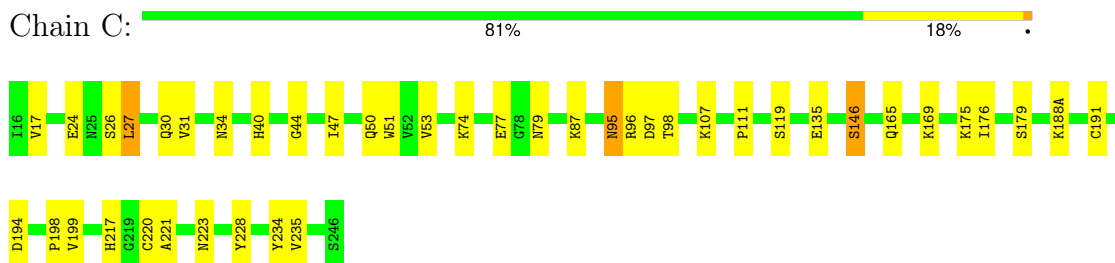
- Molecule 1: Trypsin-3



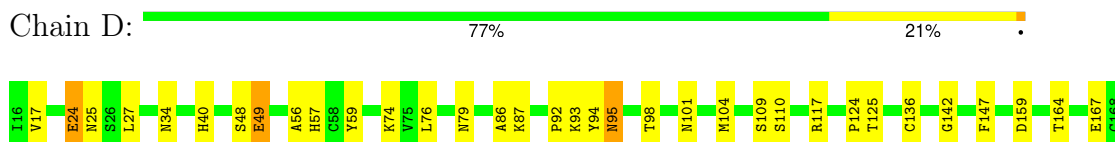
- Molecule 1: Trypsin-3



- Molecule 1: Trypsin-3

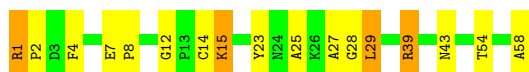


- Molecule 1: Trypsin-3

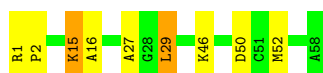
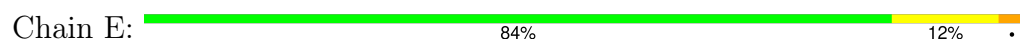




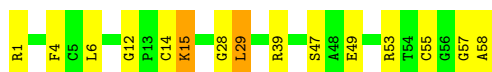
- Molecule 2: Pancreatic trypsin inhibitor



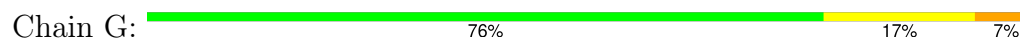
- Molecule 2: Pancreatic trypsin inhibitor



- Molecule 2: Pancreatic trypsin inhibitor



- Molecule 2: Pancreatic trypsin inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.22Å 109.72Å 81.17Å 90.00° 117.15° 90.00°	Depositor
Resolution (Å)	25.60 – 1.40 25.60 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.60-1.40) 90.2 (25.60-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.67 (at 1.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.170 , 0.224 0.173 , 0.219	Depositor DCC
R_{free} test set	1838 reflections (0.90%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.328 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9414	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.90% 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: SO4

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	1.21	1/1759 (0.1%)	1.09	3/2392 (0.1%)
1	B	1.19	3/1759 (0.2%)	1.14	5/2389 (0.2%)
1	C	1.20	0/1751	1.13	2/2380 (0.1%)
1	D	1.20	0/1757	1.17	5/2388 (0.2%)
2	E	1.17	0/465	1.22	3/622 (0.5%)
2	F	1.25	1/465 (0.2%)	1.44	6/622 (1.0%)
2	G	1.33	0/465	1.20	3/622 (0.5%)
2	I	1.28	1/465 (0.2%)	1.34	7/622 (1.1%)
All	All	1.21	6/8886 (0.1%)	1.17	34/12037 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	E	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	VAL	CA-CB	5.57	1.60	1.54
1	B	134	THR	CA-CB	5.53	1.62	1.53
1	B	121	ILE	CA-CB	5.47	1.62	1.54
2	I	43	ASN	CA-C	5.40	1.59	1.53
2	F	12	GLY	C-O	5.34	1.31	1.24
1	B	103	ILE	CA-CB	5.17	1.60	1.55

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	15	LYS	N-CA-CB	-11.77	92.09	110.92
2	F	15	LYS	CA-C-O	-8.06	110.44	119.95
2	I	1	ARG	CA-C-N	-7.68	111.87	119.78
2	I	1	ARG	C-N-CA	-7.68	111.87	119.78
1	D	27	LEU	CA-C-N	7.52	127.69	119.87
1	D	27	LEU	C-N-CA	7.52	127.69	119.87
2	F	15	LYS	CB-CA-C	7.39	122.92	111.02
2	E	15	LYS	CB-CA-C	6.64	121.95	110.72
1	D	110	SER	CA-C-N	-6.55	113.01	119.76
1	D	110	SER	C-N-CA	-6.55	113.01	119.76
2	F	15	LYS	O-C-N	6.53	130.29	122.26
1	C	169	LYS	N-CA-C	6.49	119.18	111.71
1	B	78	GLY	N-CA-C	6.41	123.61	114.64
2	E	16	ALA	N-CA-CB	6.41	119.01	110.29
2	G	15	LYS	CB-CA-C	6.33	121.29	111.28
1	A	148	GLY	N-CA-C	-6.22	100.37	110.95
1	D	24	GLU	N-CA-C	6.07	118.69	111.71
1	A	26	SER	N-CA-C	6.01	121.54	113.72
2	I	8	PRO	CA-C-N	-5.95	114.14	120.03
2	I	8	PRO	C-N-CA	-5.95	114.14	120.03
2	F	15	LYS	CA-C-N	-5.89	109.98	121.06
2	F	15	LYS	C-N-CA	-5.89	109.98	121.06
2	I	15	LYS	N-CA-CB	-5.87	102.24	111.39
2	E	15	LYS	O-C-N	-5.81	115.33	122.25
1	A	71	HIS	N-CA-C	-5.65	104.54	112.12
1	B	75	VAL	CB-CA-C	-5.57	104.91	111.09
1	B	110	SER	CA-C-N	-5.51	114.25	119.76
1	B	110	SER	C-N-CA	-5.51	114.25	119.76
2	I	12	GLY	CA-C-N	5.47	125.16	119.64
2	I	12	GLY	C-N-CA	5.47	125.16	119.64
1	B	71	HIS	N-CA-C	-5.46	104.81	112.12
2	G	7	GLU	CA-C-N	-5.42	114.80	120.38
2	G	7	GLU	C-N-CA	-5.42	114.80	120.38
1	C	146	SER	N-CA-C	-5.07	105.94	111.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	147	PHE	Peptide
2	E	15	LYS	Mainchain

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	1713	0	1670	26	0
1	B	1717	0	1672	33	0
1	C	1708	0	1659	22	0
1	D	1711	0	1664	27	0
2	E	454	0	438	6	0
2	F	454	0	438	10	1
2	G	454	0	438	10	0
2	I	454	0	438	29	1
3	A	5	0	0	0	0
3	B	25	0	0	2	0
3	C	10	0	0	0	0
3	D	20	0	0	0	0
3	E	10	0	0	0	0
3	F	15	0	0	0	0
3	G	15	0	0	0	0
3	I	5	0	0	0	0
4	A	176	0	0	5	0
4	B	129	0	0	1	1
4	C	102	0	0	3	1
4	D	101	0	0	4	0
4	E	41	0	0	2	0
4	F	31	0	0	1	0
4	G	34	0	0	1	0
4	I	30	0	0	0	0
All	All	9414	0	8417	156	2

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 9.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:LEU:HD21	4:E:76:HOH:O	1.86	0.76
2:I:29:LEU:N	2:I:29:LEU:HD23	2.02	0.75
1:A:24:GLU:HG2	1:A:117:ARG:NH2	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:ARG:HB2	2:I:2:PRO:HD3	1.75	0.69
1:B:217:HIS:HD2	3:B:14:SO4:O3	1.76	0.68
2:I:1:ARG:HB2	2:I:2:PRO:CD	2.23	0.68
4:A:404:HOH:O	1:C:24:GLU:HG3	1.95	0.67
2:I:1:ARG:N	2:I:58:ALA:HA	2.09	0.67
2:F:47:SER:HB2	2:F:49:GLU:OE1	1.95	0.66
2:I:39:ARG:HH11	2:I:39:ARG:HB3	1.61	0.65
1:B:144:THR:C	1:B:145:LEU:HD22	2.22	0.64
1:A:27[A]:LEU:HD12	1:A:29:TYR:OH	1.97	0.64
1:B:124:PRO:HD3	1:B:209:LEU:O	1.99	0.63
2:I:1:ARG:N	2:I:58:ALA:CB	2.60	0.63
2:I:39:ARG:HH11	2:I:39:ARG:CG	2.11	0.63
2:G:21:TYR:CD1	2:G:47:SER:HA	2.34	0.63
2:I:27:ALA:O	2:I:29:LEU:CD2	2.46	0.63
1:D:142:GLY:HA2	1:D:193:ARG:HB3	1.81	0.62
1:B:71:HIS:HD2	4:B:304:HOH:O	1.82	0.62
2:G:24:ASN:C	2:G:24:ASN:HD22	2.08	0.62
1:D:169:LYS:HE3	4:D:343:HOH:O	2.00	0.61
2:I:39:ARG:HH11	2:I:39:ARG:CB	2.14	0.61
1:B:95:ASN:HD22	1:B:97:ASP:H	1.49	0.61
1:B:186:GLU:HB2	1:C:135:GLU:HG3	1.82	0.60
2:I:28:GLY:C	2:I:29:LEU:HD23	2.27	0.60
1:B:145:LEU:HD22	1:B:145:LEU:N	2.17	0.59
2:E:52:MET:HE1	4:E:98:HOH:O	2.02	0.59
1:A:95:ASN:HD22	1:A:97:ASP:H	1.49	0.59
2:G:21:TYR:CE1	2:G:47:SER:HA	2.38	0.59
2:I:29:LEU:N	2:I:29:LEU:CD2	2.66	0.59
1:B:95:ASN:HD22	1:B:95:ASN:C	2.11	0.58
1:B:97:ASP:O	2:F:39:ARG:NH2	2.37	0.58
2:I:1:ARG:CB	2:I:2:PRO:HD3	2.34	0.57
2:I:28:GLY:C	2:I:29:LEU:CD2	2.77	0.57
2:E:27:ALA:HB1	2:E:29:LEU:CD2	2.35	0.57
2:E:1:ARG:N	2:E:2:PRO:HD3	2.20	0.57
2:G:49:GLU:H	2:G:49:GLU:CD	2.13	0.57
2:G:21:TYR:CE2	2:G:32:THR:HG22	2.40	0.56
1:A:222:LYS:HD2	4:A:373:HOH:O	2.05	0.56
2:I:1:ARG:CB	2:I:2:PRO:CD	2.84	0.56
2:I:27:ALA:O	2:I:29:LEU:HD23	2.06	0.55
2:F:49:GLU:CD	2:F:49:GLU:H	2.15	0.55
1:A:96:ARG:HG3	4:A:298:HOH:O	2.07	0.54
1:C:217[A]:HIS:CE1	4:C:332:HOH:O	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:NZ	1:A:217[A]:HIS:HE1	2.06	0.53
1:B:24:GLU:HB3	1:B:117:ARG:HH21	1.73	0.53
1:B:217:HIS:HE1	4:F:72:HOH:O	1.92	0.53
1:C:34:ASN:HD21	1:C:40:HIS:CE1	2.27	0.53
2:E:1:ARG:N	2:E:2:PRO:CD	2.72	0.53
2:I:1:ARG:H2	2:I:58:ALA:HA	1.73	0.53
1:A:199:VAL:HG21	1:A:228:TYR:CD2	2.44	0.53
1:D:92:PRO:HG3	4:D:307:HOH:O	2.09	0.52
2:I:39:ARG:HG3	2:I:39:ARG:NH1	2.24	0.52
1:D:79:ASN:O	4:D:339:HOH:O	2.19	0.52
1:C:199:VAL:HG21	1:C:228:TYR:CD2	2.45	0.52
2:I:1:ARG:N	2:I:58:ALA:CA	2.72	0.52
2:I:39:ARG:HH11	2:I:39:ARG:HG3	1.75	0.52
1:D:125:THR:HG23	1:D:204:GLN:HE22	1.75	0.52
2:G:29:LEU:HD21	4:G:67:HOH:O	2.10	0.52
1:A:33:LEU:HD23	1:A:33:LEU:N	2.25	0.51
2:E:1:ARG:H2	2:E:2:PRO:CD	2.23	0.51
2:G:23:TYR:CE1	2:G:25:ALA:HA	2.46	0.51
2:I:39:ARG:CG	2:I:39:ARG:NH1	2.73	0.51
1:C:31:VAL:HG22	1:C:44:GLY:C	2.35	0.51
1:D:176:ILE:HG23	1:D:180:MET:HB2	1.92	0.51
1:B:24:GLU:HB3	1:B:117:ARG:NH2	2.25	0.50
1:C:50:GLN:NE2	1:C:111:PRO:HD3	2.25	0.50
1:D:79:ASN:HB2	4:D:332:HOH:O	2.12	0.50
1:A:37:SER:HB3	4:A:322:HOH:O	2.11	0.50
1:C:95:ASN:HD22	1:C:97:ASP:H	1.60	0.50
1:B:97:ASP:O	2:F:39:ARG:NE	2.43	0.49
1:C:175:LYS:HD3	4:C:332:HOH:O	2.12	0.49
1:B:50:GLN:HG3	1:B:111:PRO:HA	1.94	0.49
1:D:124:PRO:HD3	1:D:209:LEU:O	2.12	0.49
1:D:199:VAL:HG21	1:D:228:TYR:CD2	2.48	0.49
2:I:27:ALA:C	2:I:29:LEU:HD23	2.38	0.49
1:D:164:THR:OG1	1:D:167:GLU:HG3	2.12	0.49
1:B:17:VAL:CG1	1:B:145:LEU:HD21	2.43	0.49
1:A:45:SER:OG	1:A:198:PRO:HB3	2.13	0.48
1:C:47:ILE:HD13	1:C:53:VAL:HG23	1.95	0.48
1:D:24:GLU:HG2	1:D:117:ARG:NH2	2.28	0.48
1:D:124:PRO:HA	1:D:204:GLN:OE1	2.13	0.48
1:B:217:HIS:CD2	3:B:14:SO4:O3	2.62	0.48
1:A:134:THR:O	1:A:161:PRO:HA	2.13	0.48
1:A:24:GLU:OE2	1:A:117:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:CYS:O	1:C:221:ALA:HB3	2.13	0.48
1:B:95:ASN:ND2	1:B:98:THR:H	2.12	0.47
1:B:95:ASN:ND2	1:B:97:ASP:H	2.10	0.47
1:B:17:VAL:HG22	1:B:145:LEU:HD22	1.96	0.47
1:D:56:ALA:HA	1:D:104:MET:HB2	1.97	0.47
1:D:241:THR:O	1:D:245:ASN:HB2	2.15	0.47
2:I:1:ARG:H1	2:I:58:ALA:HA	1.76	0.47
1:A:95:ASN:ND2	1:A:97:ASP:H	2.13	0.46
1:D:232:TYR:O	1:D:235:VAL:HG23	2.15	0.46
1:A:175:LYS:HZ1	1:A:217[A]:HIS:HE1	1.62	0.46
2:G:1:ARG:H1	2:G:58:ALA:HA	1.78	0.46
2:G:4:PHE:C	2:G:4:PHE:CD1	2.93	0.46
1:A:142:GLY:HA2	1:A:193:ARG:HB3	1.98	0.46
1:B:128:PRO:HG3	1:B:232:TYR:CE2	2.51	0.46
1:D:49:GLU:H	1:D:49:GLU:CD	2.23	0.46
1:B:45:SER:OG	1:B:198:PRO:HB3	2.16	0.45
1:B:173:PRO:O	1:B:175:LYS:HD2	2.15	0.45
1:C:191:CYS:O	1:C:194:ASP:HB2	2.16	0.45
1:C:217[A]:HIS:HE1	4:C:332:HOH:O	1.95	0.45
1:B:17:VAL:HG13	1:B:145:LEU:HD21	1.98	0.45
2:I:1:ARG:H2	2:I:58:ALA:CA	2.30	0.45
2:I:27:ALA:O	2:I:29:LEU:HD21	2.15	0.45
1:B:61:THR:HG22	1:B:62:ARG:HD2	1.98	0.44
1:A:213:VAL:HG22	1:A:228:TYR:HE2	1.82	0.44
1:B:51:TRP:CH2	1:B:107:LYS:HB2	2.53	0.44
1:B:213:VAL:HA	1:B:228:TYR:CD2	2.53	0.44
2:F:4:PHE:C	2:F:4:PHE:CD1	2.96	0.44
1:D:76:LEU:HD12	1:D:76:LEU:N	2.33	0.44
1:D:34:ASN:HD21	1:D:40:HIS:CE1	2.36	0.43
1:B:17:VAL:O	1:B:188(A):LYS:HA	2.18	0.43
1:C:50:GLN:HE22	1:C:111:PRO:HD3	1.82	0.43
1:D:195:ALA:HB2	2:I:15:LYS:C	2.43	0.43
1:D:95:ASN:ND2	1:D:98:THR:H	2.16	0.43
1:C:165:GLN:HE22	1:C:176:ILE:HG21	1.84	0.43
1:D:57:HIS:CD2	2:I:14:CYS:HB3	2.53	0.43
2:F:28:GLY:O	2:F:29:LEU:CD1	2.67	0.43
2:F:1:ARG:N	2:F:58:ALA:HA	2.34	0.43
1:A:145:LEU:HD21	4:A:263:HOH:O	2.19	0.43
1:B:195:ALA:HB2	2:F:15:LYS:C	2.43	0.43
1:A:158:LEU:HD11	1:A:188(A):LYS:HB3	2.00	0.43
1:B:57:HIS:CD2	2:F:14:CYS:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:ARG:N	2:G:58:ALA:HA	2.34	0.42
1:A:211:GLY:HA2	1:A:229:THR:O	2.18	0.42
1:C:51:TRP:CZ2	1:C:107:LYS:HD2	2.54	0.42
1:D:136:CYS:O	1:D:159:ASP:HA	2.20	0.42
1:B:142:GLY:HA2	1:B:193:ARG:HB3	2.01	0.42
2:I:23:TYR:CE1	2:I:25:ALA:HA	2.55	0.42
1:A:217[B]:HIS:CE1	1:A:221(A):TRP:CZ3	3.07	0.42
1:C:95:ASN:ND2	1:C:98:THR:H	2.17	0.42
2:F:55:CYS:O	2:F:58:ALA:HB2	2.20	0.42
1:A:32:SER:C	1:A:33:LEU:HD23	2.45	0.42
1:B:191:CYS:O	1:B:194:ASP:HB2	2.19	0.42
1:D:17:VAL:O	1:D:188(A):LYS:HA	2.20	0.42
1:D:181:PHE:CE2	1:D:183:VAL:CG2	3.03	0.42
1:B:137:LEU:HD11	1:B:157:CYS:HB3	2.02	0.42
1:A:24:GLU:CG	1:A:117:ARG:NH2	2.78	0.41
1:D:86:ALA:HB2	1:D:109:SER:HA	2.02	0.41
1:A:95:ASN:ND2	1:A:98:THR:H	2.19	0.41
1:C:26:SER:C	1:C:27:LEU:HD23	2.45	0.41
2:I:4:PHE:HA	2:I:7:GLU:HG2	2.02	0.41
1:C:87:LYS:HD2	1:C:107:LYS:HD3	2.03	0.41
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.55	0.41
1:C:30:GLN:HE22	1:C:198:PRO:HD2	1.86	0.41
1:C:179:SER:HB2	1:C:234:TYR:OH	2.20	0.41
1:A:82:PHE:CD2	1:A:82:PHE:N	2.89	0.41
1:B:17:VAL:HG13	1:B:145:LEU:CD2	2.51	0.40
1:A:137:LEU:HD11	1:A:157:CYS:HB3	2.03	0.40
1:C:17:VAL:O	1:C:188(A):LYS:HA	2.21	0.40
1:D:94:TYR:HA	1:D:101:ASN:HB2	2.03	0.40
2:I:28:GLY:C	2:I:29:LEU:HD22	2.46	0.40
1:D:59:TYR:CD2	1:D:59:TYR:C	3.00	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:54:THR:O	2:F:53:ARG:NH1[1_556]	2.10	0.10
4:B:270:HOH:O	4:C:287:HOH:O[2_454]	2.19	0.01

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	224/224 (100%)	217 (97%)	7 (3%)	0	100	100
1	B	225/224 (100%)	212 (94%)	12 (5%)	1 (0%)	30	11
1	C	223/224 (100%)	215 (96%)	8 (4%)	0	100	100
1	D	224/224 (100%)	214 (96%)	10 (4%)	0	100	100
2	E	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
2	F	56/58 (97%)	54 (96%)	1 (2%)	1 (2%)	7	0
2	G	56/58 (97%)	53 (95%)	2 (4%)	1 (2%)	7	0
2	I	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
All	All	1120/1128 (99%)	1073 (96%)	44 (4%)	3 (0%)	37	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	LEU
2	G	57	GLY
2	F	57	GLY

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	187/185 (101%)	175 (94%)	12 (6%)	14	1
1	B	187/185 (101%)	178 (95%)	9 (5%)	21	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	186/185 (100%)	176 (95%)	10 (5%)	18	2
1	D	187/185 (101%)	179 (96%)	8 (4%)	25	3
2	E	46/46 (100%)	43 (94%)	3 (6%)	14	1
2	F	46/46 (100%)	44 (96%)	2 (4%)	25	3
2	G	46/46 (100%)	42 (91%)	4 (9%)	8	0
2	I	46/46 (100%)	44 (96%)	2 (4%)	25	3
All	All	931/924 (101%)	881 (95%)	50 (5%)	18	2

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	50	GLN
1	A	61	THR
1	A	62	ARG
1	A	95	ASN
1	A	96	ARG
1	A	110	SER
1	A	117	ARG
1	A	138	ILE
1	A	161	PRO
1	A	169	LYS
1	A	235	VAL
1	B	50	GLN
1	B	77	GLU
1	B	95	ASN
1	B	97	ASP
1	B	110	SER
1	B	117	ARG
1	B	145	LEU
1	B	165	GLN
1	B	175	LYS
1	C	27	LEU
1	C	74	LYS
1	C	77	GLU
1	C	79	ASN
1	C	95	ASN
1	C	96	ARG
1	C	119	SER
1	C	146	SER

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Mol	Chain	Res	Type
1	C	223	ASN
1	C	235	VAL
1	D	25	ASN
1	D	48	SER
1	D	49	GLU
1	D	74	LYS
1	D	87	LYS
1	D	93	LYS
1	D	95	ASN
1	D	175	LYS
2	I	29	LEU
2	I	39	ARG
2	E	29	LEU
2	E	46	LYS
2	E	50	ASP
2	F	6	LEU
2	F	29	LEU
2	G	1	ARG
2	G	24	ASN
2	G	29	LEU
2	G	49	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	50	GLN
1	A	64	GLN
1	A	84	ASN
1	A	95	ASN
1	B	50	GLN
1	B	71	HIS
1	B	84	ASN
1	B	95	ASN
1	B	165	GLN
1	B	204	GLN
1	B	217	HIS
1	B	245	ASN
1	C	30	GLN
1	C	34	ASN
1	C	50	GLN
1	C	95	ASN

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Mol	Chain	Res	Type
1	C	165	GLN
1	C	223	ASN
1	D	34	ASN
1	D	95	ASN
1	D	223	ASN
2	I	31	GLN
2	F	31	GLN
2	G	24	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	C	1	-	4,4,4	0.55	0	6,6,6	0.76	0
3	SO4	G	61	-	4,4,4	0.67	0	6,6,6	0.34	0
3	SO4	C	247	-	4,4,4	0.88	0	6,6,6	0.75	0
3	SO4	E	59	-	4,4,4	0.30	0	6,6,6	0.78	0
3	SO4	G	60	-	4,4,4	0.45	0	6,6,6	0.85	0
3	SO4	D	8	-	4,4,4	0.29	0	6,6,6	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	59	-	4,4,4	0.45	0	6,6,6	0.93	0
3	SO4	D	15	-	4,4,4	0.51	0	6,6,6	0.53	0
3	SO4	B	6	-	4,4,4	0.44	0	6,6,6	0.78	0
3	SO4	B	247[B]	-	4,4,4	0.29	0	6,6,6	0.20	0
3	SO4	D	247	-	4,4,4	0.59	0	6,6,6	1.87	1 (16%)
3	SO4	E	60	-	4,4,4	0.50	0	6,6,6	0.80	0
3	SO4	F	61	-	4,4,4	0.49	0	6,6,6	0.37	0
3	SO4	B	247[A]	-	4,4,4	0.28	0	6,6,6	0.62	0
3	SO4	B	14	-	4,4,4	0.37	0	6,6,6	0.57	0
3	SO4	A	7	-	4,4,4	0.42	0	6,6,6	0.54	0
3	SO4	B	13	-	4,4,4	0.18	0	6,6,6	0.91	0
3	SO4	I	59	-	4,4,4	0.58	0	6,6,6	1.23	0
3	SO4	D	248	-	4,4,4	0.79	0	6,6,6	0.91	0
3	SO4	G	59	-	4,4,4	0.61	0	6,6,6	0.87	0
3	SO4	F	60	-	4,4,4	0.35	0	6,6,6	0.51	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	247	SO4	O4-S-O2	-3.34	92.08	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	14	SO4	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	224/224 (100%)	-0.99	0 100 100	11, 19, 29, 41	7 (3%)
1	B	224/224 (100%)	-0.92	0 100 100	11, 21, 32, 41	8 (3%)
1	C	224/224 (100%)	-0.88	0 100 100	11, 22, 35, 78	4 (1%)
1	D	224/224 (100%)	-0.92	0 100 100	11, 22, 33, 47	6 (2%)
2	E	58/58 (100%)	-0.91	0 100 100	14, 20, 30, 38	2 (3%)
2	F	58/58 (100%)	-0.84	0 100 100	15, 21, 34, 41	4 (6%)
2	G	58/58 (100%)	-0.70	0 100 100	14, 23, 37, 46	5 (8%)
2	I	58/58 (100%)	-0.90	0 100 100	16, 22, 34, 45	2 (3%)
All	All	1128/1128 (100%)	-0.91	0 100 100	11, 21, 33, 78	38 (3%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
3	SO4	C	247	5/5	0.97	0.06	36,39,53,79	0
3	SO4	D	248	5/5	0.97	0.05	29,35,51,70	0
3	SO4	D	15	5/5	0.98	0.05	38,47,63,74	0
3	SO4	D	247	5/5	0.98	0.05	25,40,47,55	0
3	SO4	B	14	5/5	0.98	0.05	35,45,53,61	0
3	SO4	I	59	5/5	0.98	0.04	31,32,36,41	0
3	SO4	E	60	5/5	0.98	0.04	30,32,40,48	0
3	SO4	G	59	5/5	0.98	0.06	24,32,35,41	0
3	SO4	G	60	5/5	0.98	0.05	25,26,44,49	0
3	SO4	G	61	5/5	0.98	0.04	43,44,56,73	0
3	SO4	B	247[A]	5/5	0.99	0.04	18,23,24,25	5
3	SO4	B	247[B]	5/5	0.99	0.04	20,23,30,32	5
3	SO4	E	59	5/5	0.99	0.03	20,21,24,27	0
3	SO4	B	6	5/5	0.99	0.03	31,35,39,41	0
3	SO4	F	59	5/5	0.99	0.03	20,27,29,35	0
3	SO4	F	60	5/5	0.99	0.04	27,28,31,39	0
3	SO4	F	61	5/5	0.99	0.04	35,38,43,43	0
3	SO4	D	8	5/5	0.99	0.04	30,31,38,40	0
3	SO4	B	13	5/5	0.99	0.04	33,35,39,51	0
3	SO4	A	7	5/5	0.99	0.04	34,38,40,51	0
3	SO4	C	1	5/5	1.00	0.02	21,21,25,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.