



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 PM UTC

PDB ID : 3KSE / pdb_00003kse
Title : Unreduced cathepsin L in complex with stefin A
Authors : Renko, M.; Turk, D.
Deposited on : 2009-11-22
Resolution : 1.71 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

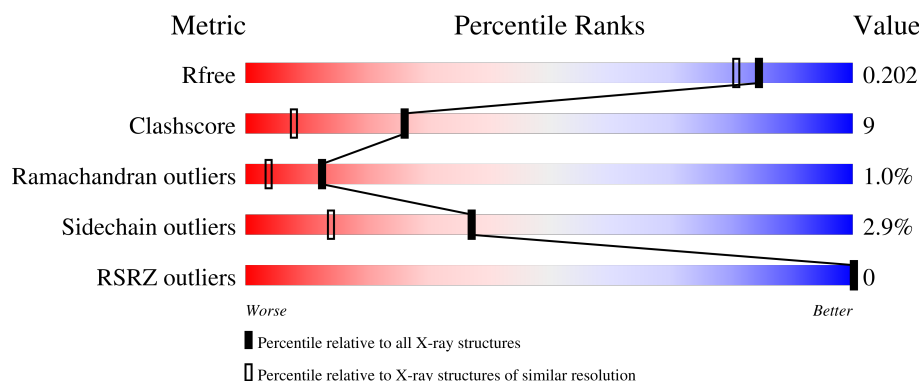
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	220	76% 22% .
1	B	220	79% 19% .
1	C	220	81% 18% .
2	D	98	81% 17% .
2	E	98	80% 19% .

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Mol	Chain	Length	Quality of chain
2	F	98	 78% 20% ..

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
1	SCH	A	25	-	-	X	-
1	SCH	B	25[A]	-	-	X	-
1	SCH	B	25[B]	-	-	X	-
1	SCH	C	25[A]	-	-	X	-
1	SCH	C	25[B]	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8650 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 Cathepsin L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	12	9	0
			1736	1088	285	347	16			
1	B	220	Total	C	N	O	S	7	6	0
			1720	1076	281	346	17			
1	C	220	Total	C	N	O	S	8	7	0
			1721	1077	281	345	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	THR	engineered mutation	UNP P07711
A	179	ASP	ASN	engineered mutation	UNP P07711
B	110	ALA	THR	engineered mutation	UNP P07711
B	179	ASP	ASN	engineered mutation	UNP P07711
C	110	ALA	THR	engineered mutation	UNP P07711
C	179	ASP	ASN	engineered mutation	UNP P07711

- Molecule 2 is a protein called Cystatin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	98	Total	C	N	O	S	6	0	0
			775	492	126	155	2			
2	E	98	Total	C	N	O	S	0	0	0
			775	492	126	155	2			
2	F	98	Total	C	N	O	S	0	1	0
			780	496	127	155	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	261	Total	O	0	0
			261	261		

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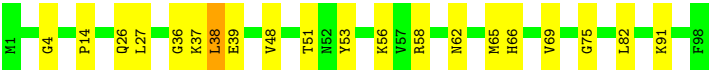
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	276	Total 276	O 276	0	0
3	C	269	Total 269	O 269	0	0
3	D	112	Total 112	O 112	0	0
3	E	116	Total 116	O 116	0	0
3	F	109	Total 109	O 109	0	0

Chain E:

80%

19%

.



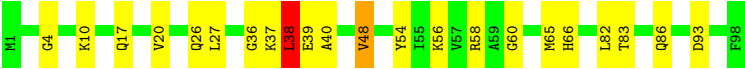
● Molecule 2: Cystatin-A

Chain F:

78%

20%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	35.23Å 83.95Å 83.91Å 118.07° 98.04° 98.04°	Depositor
Resolution (Å)	15.33 – 1.71 15.33 – 1.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.33-1.71) 95.6 (15.33-1.71)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.71Å)	Xtriage
Refinement program	MAIN	Depositor
R, R_{free}	0.153 , 0.204 0.151 , 0.202	Depositor DCC
R_{free} test set	4292 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.478 for h,l,-h-k-l 0.478 for h,-h-k-l,k 0.016 for -h,-k,h+k+l 0.017 for -h,h+k+l,-l 0.016 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8650	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.40	11/1801 (0.6%)	1.23	11/2432 (0.5%)
1	B	1.43	5/1769 (0.3%)	1.34	15/2388 (0.6%)
1	C	1.45	3/1774 (0.2%)	1.31	6/2394 (0.3%)
2	D	1.46	6/788 (0.8%)	1.34	3/1062 (0.3%)
2	E	1.39	4/788 (0.5%)	1.38	1/1062 (0.1%)
2	F	1.42	4/797 (0.5%)	1.38	3/1074 (0.3%)
All	All	1.43	33/7717 (0.4%)	1.32	39/10412 (0.4%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	GLY	C-O	-7.56	1.15	1.23
2	D	69	VAL	CA-CB	7.56	1.63	1.54
1	A	153	GLU	C-O	-6.90	1.18	1.25
1	A	205	ARG	C-O	-6.87	1.15	1.23
1	B	78	GLN	C-O	6.07	1.31	1.24
1	C	58	GLY	CA-C	5.92	1.55	1.51
2	D	81	VAL	CA-CB	5.92	1.62	1.54
1	A	101	ASN	C-O	-5.72	1.20	1.25
1	A	144	LEU	C-O	5.71	1.30	1.24
2	F	20	VAL	CA-CB	-5.62	1.47	1.54
2	E	51	THR	CA-CB	5.59	1.63	1.53
1	A	127	ALA	CA-CB	5.58	1.62	1.53
1	A	206[A]	ARG	C-O	-5.52	1.16	1.23
1	A	206[B]	ARG	C-O	-5.52	1.16	1.23
2	F	83	THR	C-O	5.52	1.31	1.24
1	C	126	VAL	C-O	-5.49	1.17	1.24
2	D	53	TYR	CA-C	-5.49	1.46	1.52
2	F	86	GLN	C-O	-5.48	1.17	1.24
1	C	126	VAL	CA-CB	-5.47	1.47	1.54
1	A	154	PRO	C-O	-5.42	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9	ALA	C-O	5.36	1.30	1.23
1	B	165	VAL	CA-CB	5.32	1.61	1.54
2	E	69	VAL	CA-CB	5.29	1.60	1.54
2	D	51	THR	CA-CB	5.24	1.63	1.53
2	D	2	ILE	CA-CB	5.22	1.59	1.55
2	F	93	ASP	N-CA	5.21	1.52	1.46
1	B	18	ASN	C-O	-5.18	1.17	1.24
1	B	135	ALA	CA-C	5.08	1.58	1.52
1	A	53	LEU	C-O	-5.08	1.18	1.24
1	A	132	ILE	CA-CB	5.06	1.61	1.54
2	E	91	LYS	N-CA	-5.03	1.40	1.46
2	E	53	TYR	N-CA	5.03	1.52	1.46
1	A	77	VAL	CA-CB	-5.01	1.48	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	PRO	N-CA-C	9.22	131.47	112.47
1	B	176	GLU	N-CA-C	7.81	120.55	111.02
1	B	175	THR	N-CA-C	7.78	120.23	109.18
2	F	38	LEU	N-CA-C	-6.80	95.95	107.99
2	E	38	LEU	N-CA-C	-6.79	97.45	108.52
1	B	58	GLY	O-C-N	-6.69	118.66	121.07
1	A	90	PRO	N-CA-C	6.68	121.43	111.41
2	D	35	TYR	N-CA-C	6.66	122.38	113.72
1	A	49	SER	N-CA-C	6.61	119.06	108.41
1	A	56	CYS	N-CA-C	6.16	121.72	113.72
1	B	49	SER	N-CA-C	6.01	118.09	108.41
1	B	67	GLY	N-CA-C	5.92	118.08	112.04
2	D	38	LEU	N-CA-C	-5.87	98.95	108.52
1	C	79	ASP	N-CA-C	5.78	117.58	111.28
1	A	104	TYR	N-CA-C	5.73	119.25	112.72
1	B	90	PRO	N-CA-C	5.60	119.81	111.41
1	B	36	GLY	CA-C-O	-5.58	114.75	120.66
1	C	2	PRO	CA-C-N	-5.51	112.47	120.29
1	C	2	PRO	C-N-CA	-5.51	112.47	120.29
1	B	159	GLU	CA-C-N	-5.36	115.20	123.14
1	B	159	GLU	C-N-CA	-5.36	115.20	123.14
1	B	104	TYR	N-CA-C	5.36	119.51	112.92
1	B	2	PRO	CA-C-N	5.34	131.31	121.70
1	B	2	PRO	C-N-CA	5.34	131.31	121.70
1	A	67	GLY	N-CA-C	5.30	117.45	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	47	VAL	CB-CA-C	-5.23	104.35	111.15
1	C	90	PRO	N-CA-C	5.21	119.23	111.41
1	A	128	THR	N-CA-C	5.18	119.88	113.50
2	F	48	VAL	CA-C-O	-5.17	114.32	120.78
1	A	159	GLU	CA-C-N	-5.14	115.53	123.14
1	A	159	GLU	C-N-CA	-5.14	115.53	123.14
2	F	54	TYR	N-CA-C	-5.10	100.41	108.73
1	B	108	ASN	CB-CA-C	-5.09	101.14	110.62
1	B	175	THR	CA-C-N	5.09	127.87	120.79
1	B	175	THR	C-N-CA	5.09	127.87	120.79
1	A	1	ALA	CA-C-N	5.06	126.17	119.84
1	A	1	ALA	C-N-CA	5.06	126.17	119.84
1	C	35	GLU	N-CA-C	-5.03	105.79	111.28
1	A	180	ASN	CB-CA-C	-5.03	101.10	109.55

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	1736	0	1614	27	0
1	B	1720	0	1596	42	0
1	C	1721	0	1600	42	0
2	D	775	0	780	9	0
2	E	775	0	780	10	0
2	F	780	0	789	13	0
3	A	261	0	0	2	1
3	B	276	0	0	2	1
3	C	269	0	0	4	0
3	D	112	0	0	1	0
3	E	116	0	0	1	0
3	F	109	0	0	2	0
All	All	8650	0	7159	137	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLN:HE22	1:C:25[B]:SCH:CE	1.49	1.26
1:C:19:GLN:NE2	1:C:25[B]:SCH:HE3	1.53	1.21
1:C:19:GLN:HE22	1:C:25[B]:SCH:HE3	0.86	1.02
1:C:19:GLN:NE2	1:C:25[B]:SCH:CE	2.19	0.95
1:A:175:THR:HG22	1:A:180:ASN:OD1	1.68	0.93
1:B:25[B]:SCH:HE2	1:B:163:HIS:CD2	2.05	0.91
1:B:175:THR:CG2	1:B:176:GLU:H	1.83	0.91
1:B:175:THR:HG22	1:B:176:GLU:H	1.40	0.86
1:B:25[B]:SCH:CE	1:B:163:HIS:CD2	2.62	0.83
1:B:175:THR:HG22	1:B:176:GLU:N	1.99	0.76
1:B:25[B]:SCH:CE	1:B:163:HIS:HD2	2.00	0.74
2:D:17:GLN:HE22	2:D:40:ALA:H	1.34	0.74
1:B:41:LYS:HG3	1:B:220:VAL:HG23	1.70	0.73
2:F:17:GLN:HE22	2:F:40:ALA:H	1.37	0.73
1:C:23:GLY:HA2	1:C:25[B]:SCH:HE1	1.69	0.72
1:A:25:SCH:HE2	1:A:163:HIS:ND1	2.03	0.72
1:C:23:GLY:HA2	1:C:25[B]:SCH:CE	2.19	0.72
1:A:175:THR:HG21	1:A:179:ASP:O	1.89	0.72
2:E:26:GLN:HE22	2:E:82:LEU:H	1.37	0.72
1:C:51:GLN:NE2	1:C:92:GLU:H	1.87	0.71
1:B:23:GLY:HA2	1:B:25[A]:SCH:CE	2.20	0.71
1:C:23:GLY:C	1:C:25[B]:SCH:HE2	2.15	0.71
1:B:23:GLY:HA2	1:B:25[A]:SCH:HE1	1.73	0.70
1:B:153:GLU:H	1:B:208:HIS:HE1	1.40	0.70
2:E:26:GLN:NE2	2:E:82:LEU:H	1.90	0.69
1:B:153:GLU:H	1:B:208:HIS:CE1	2.12	0.67
1:B:23:GLY:C	1:B:25[A]:SCH:HE2	2.20	0.67
2:F:26:GLN:NE2	2:F:82:LEU:H	1.93	0.67
1:A:12:TYR:CE2	1:A:40:ARG:HG3	2.31	0.65
2:D:26:GLN:NE2	2:D:82:LEU:H	1.93	0.65
2:D:26:GLN:HE22	2:D:82:LEU:H	1.45	0.65
1:A:153:GLU:H	1:A:208:HIS:CE1	2.15	0.65
1:C:24:SER:N	1:C:25[B]:SCH:HE2	2.12	0.64
1:C:120:LYS:NZ	3:C:276:HOH:O	2.25	0.64
2:D:65:MET:HE3	2:D:87:VAL:HG12	1.79	0.64
1:B:178:ASP:HA	3:B:574:HOH:O	1.98	0.64
2:D:17:GLN:NE2	2:D:40:ALA:H	1.96	0.63
2:F:27:LEU:HD23	2:F:38:LEU:HD21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:SER:HB3	3:C:865:HOH:O	1.97	0.63
1:C:195[B]:MET:HE1	1:C:200:LYS:HE3	1.81	0.63
1:C:25[B]:SCH:CE	1:C:25[B]:SCH:H	2.12	0.62
1:C:25[B]:SCH:HE2	1:C:25[B]:SCH:H	1.64	0.62
2:F:26:GLN:HE22	2:F:82:LEU:H	1.46	0.62
2:F:17:GLN:NE2	2:F:40:ALA:H	1.97	0.62
1:B:25[B]:SCH:HE2	1:B:163:HIS:HD2	1.55	0.62
1:B:25[A]:SCH:HE3	1:B:25[A]:SCH:H	1.66	0.61
1:A:78:GLN:HG2	3:A:987:HOH:O	2.00	0.61
2:F:39:GLU:OE2	2:F:58:ARG:NH1	2.34	0.60
1:C:2:PRO:HD2	3:C:812:HOH:O	2.01	0.59
1:B:25[B]:SCH:HE3	1:B:163:HIS:CD2	2.38	0.59
1:A:44:ARG:CZ	1:A:46:ILE:HD11	2.33	0.58
1:C:19:GLN:NE2	1:C:25[B]:SCH:HE1	2.12	0.58
1:B:52:ASN:ND2	1:B:84:ASP:H	2.03	0.57
1:C:101:ASN:C	1:C:101:ASN:HD22	2.12	0.57
1:C:51:GLN:HE21	1:C:92:GLU:H	1.50	0.57
2:D:27:LEU:HD23	2:D:38:LEU:HD11	1.87	0.56
1:A:175:THR:HG21	1:A:179:ASP:C	2.31	0.56
1:B:192[A]:GLU:OE2	2:E:75:GLY:HA3	2.05	0.56
1:A:18:ASN:ND2	1:A:20:GLY:H	2.03	0.55
2:E:66:HIS:HD2	3:E:171:HOH:O	1.90	0.54
1:C:52:ASN:ND2	1:C:84:ASP:H	2.06	0.54
2:E:38:LEU:HD21	2:E:65:MET:HE1	1.89	0.53
1:B:41:LYS:HG3	1:B:220:VAL:CG2	2.38	0.52
1:B:8:ARG:NH2	1:B:184:LEU:HD21	2.24	0.52
1:C:124[B]:LYS:HE2	3:C:452:HOH:O	2.09	0.52
2:F:27:LEU:CD2	2:F:38:LEU:HD21	2.39	0.52
2:D:66:HIS:HD2	3:D:111:HOH:O	1.93	0.51
1:A:18:ASN:HD22	1:A:20:GLY:H	1.56	0.51
1:A:108[A]:ASN:ND2	3:A:853:HOH:O	2.42	0.51
1:B:175:THR:HG23	1:B:176:GLU:H	1.74	0.51
1:C:152:PHE:HA	1:C:208:HIS:CE1	2.44	0.51
1:C:71:ASP:O	1:C:75:GLN:HG3	2.09	0.51
1:B:178:ASP:HB2	1:C:206:ARG:HG3	1.92	0.51
1:A:175:THR:HG23	1:A:178:ASP:N	2.25	0.51
1:B:140:HIS:HE1	1:B:155:ASP:OD1	1.94	0.50
2:E:56:LYS:NZ	2:E:66:HIS:HE1	2.09	0.50
1:C:7:TRP:CE2	1:C:130:GLY:HA2	2.47	0.50
2:F:10[B]:LYS:NZ	3:F:1102:HOH:O	2.44	0.50
2:F:66:HIS:HD2	3:F:107:HOH:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HD22	1:A:18:ASN:C	2.20	0.50
1:B:25[A]:SCH:CE	1:B:25[A]:SCH:H	2.24	0.50
1:C:23:GLY:CA	1:C:25[B]:SCH:HE2	2.43	0.49
1:A:25:SCH:CE	1:A:163:HIS:ND1	2.75	0.49
1:C:23:GLY:HA2	1:C:25[B]:SCH:HE2	1.94	0.48
1:B:219:THR:HG21	3:B:934:HOH:O	2.13	0.48
1:C:25[A]:SCH:CE	1:C:163:HIS:ND1	2.76	0.48
2:F:38:LEU:HD11	2:F:65:MET:CE	2.43	0.48
1:B:177:SER:O	1:B:178:ASP:HB2	2.13	0.48
1:C:177:SER:O	1:C:178:ASP:HB2	2.14	0.48
1:C:101:ASN:HD22	1:C:102:PRO:HD2	1.80	0.47
1:B:163:HIS:HE1	1:B:187:ASN:OD1	1.97	0.47
2:D:27:LEU:HD11	2:D:65:MET:HE1	1.97	0.47
1:B:175:THR:H	1:B:180:ASN:ND2	2.12	0.47
1:C:117:LYS:HG2	1:C:213:SER:HA	1.95	0.47
1:C:101:ASN:HD22	1:C:102:PRO:N	2.13	0.47
1:B:123:MET:HE3	1:B:170:TYR:CE1	2.49	0.47
1:A:25:SCH:HE1	2:D:47:VAL:O	2.15	0.46
1:B:23:GLY:CA	1:B:25[A]:SCH:HE2	2.45	0.46
1:A:40:ARG:HD2	1:A:129:VAL:O	2.15	0.46
1:C:44:ARG:CZ	1:C:46:ILE:HD11	2.46	0.46
2:E:27:LEU:HD23	2:E:38:LEU:HD11	1.97	0.46
1:A:69:LEU:HD12	1:A:72:TYR:CZ	2.51	0.45
1:B:23:GLY:HA2	1:B:25[A]:SCH:HE2	1.95	0.45
1:B:23:GLY:CA	1:B:25[A]:SCH:CE	2.93	0.45
1:C:101:ASN:HD22	1:C:102:PRO:CD	2.29	0.45
1:A:8:ARG:HD3	1:A:198:TYR:CZ	2.52	0.45
1:A:113:VAL:HG23	1:A:219[B]:THR:CG2	2.47	0.45
1:A:71:ASP:O	1:A:75:GLN:HG3	2.17	0.45
1:B:52:ASN:HD22	1:B:84:ASP:HB2	1.82	0.44
1:B:19:GLN:OE1	1:B:25[A]:SCH:HE3	2.17	0.44
1:A:25:SCH:HE2	1:A:163:HIS:CE1	2.52	0.44
1:C:117:LYS:HE3	1:C:213:SER:O	2.18	0.44
1:C:8:ARG:HD3	1:C:198:TYR:CZ	2.52	0.44
1:B:7:TRP:CE2	1:B:130:GLY:HA2	2.54	0.43
1:C:25[A]:SCH:HE2	1:C:163:HIS:ND1	2.34	0.43
1:A:7:TRP:CE2	1:A:130:GLY:HA2	2.53	0.43
2:F:56:LYS:NZ	2:F:66:HIS:HE1	2.17	0.43
1:C:25[B]:SCH:SD	2:F:4:GLY:HA2	2.59	0.42
1:A:12:TYR:HE2	1:A:40:ARG:HG3	1.79	0.42
1:B:23:GLY:C	1:B:25[A]:SCH:CE	2.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25[B]:SCH:SD	2:E:4:GLY:HA2	2.59	0.42
1:C:19:GLN:HE22	1:C:25[B]:SCH:HE1	1.60	0.42
1:C:25[A]:SCH:HE3	1:C:163:HIS:ND1	2.35	0.42
1:C:25[A]:SCH:SD	2:F:4:GLY:HA2	2.60	0.42
1:C:177:SER:O	1:C:178:ASP:CB	2.68	0.42
1:C:101:ASN:ND2	1:C:103:LYS:H	2.18	0.41
1:A:152:PHE:HA	1:A:208:HIS:NE2	2.35	0.41
1:B:8:ARG:HD3	1:B:198:TYR:CZ	2.55	0.41
2:E:39:GLU:OE2	2:E:58:ARG:NH2	2.50	0.41
1:A:175:THR:HG23	1:A:178:ASP:H	1.85	0.41
1:C:58:GLY:N	1:C:59:PRO:CD	2.83	0.41
1:A:58:GLY:N	1:A:59:PRO:CD	2.83	0.41
1:B:177:SER:O	1:B:178:ASP:CB	2.68	0.40
2:E:56:LYS:HZ3	2:E:66:HIS:HE1	1.70	0.40
1:B:163:HIS:CE1	1:B:187:ASN:OD1	2.74	0.40
1:A:52:ASN:HD22	1:A:52:ASN:C	2.29	0.40
1:B:152:PHE:HA	1:B:208:HIS:NE2	2.36	0.40

All (1) 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)
3:A:861:HOH:O	3:B:471:HOH:O[1_554]	2.18	0.02

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	226/220 (103%)	221 (98%)	4 (2%)	1 (0%)	30	16
1	B	222/220 (101%)	215 (97%)	6 (3%)	1 (0%)	24	11
1	C	223/220 (101%)	218 (98%)	4 (2%)	1 (0%)	30	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	96/98 (98%)	93 (97%)	2 (2%)	1 (1%)	12	4
2	E	96/98 (98%)	92 (96%)	2 (2%)	2 (2%)	5	1
2	F	97/98 (99%)	92 (95%)	2 (2%)	3 (3%)	3	0
All	All	960/954 (101%)	931 (97%)	20 (2%)	9 (1%)	12	4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	B	2	PRO
1	C	2	PRO
2	F	60	GLY
2	E	36	GLY
2	F	36	GLY
2	E	48	VAL
2	F	48	VAL
2	D	48	VAL

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	186/177 (105%)	180 (97%)	6 (3%)	34	11
1	B	182/177 (103%)	176 (97%)	6 (3%)	33	10
1	C	183/177 (103%)	177 (97%)	6 (3%)	33	10
2	D	85/85 (100%)	84 (99%)	1 (1%)	63	46
2	E	85/85 (100%)	82 (96%)	3 (4%)	32	9
2	F	86/85 (101%)	84 (98%)	2 (2%)	44	21
All	All	807/786 (103%)	783 (97%)	24 (3%)	37	12

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	34[A]	LEU
1	A	34[B]	LEU
1	A	116	PRO
1	A	156	CYS
1	A	159	GLU
1	B	116	PRO
1	B	117	LYS
1	B	156	CYS
1	B	159	GLU
1	B	199	VAL
1	B	220	VAL
1	C	2	PRO
1	C	15	PRO
1	C	116	PRO
1	C	120	LYS
1	C	148	GLU
1	C	156	CYS
2	D	39	GLU
2	E	14	PRO
2	E	37	LYS
2	E	62	ASN
2	F	37	LYS
2	F	38	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	19	GLN
1	A	60	GLN
1	A	66	ASN
1	A	208	HIS
1	B	21	GLN
1	B	52	ASN
1	B	80	ASN
1	B	140	HIS
1	B	163	HIS
1	B	180	ASN
1	B	208	HIS
1	C	19	GLN
1	C	21	GLN
1	C	51	GLN

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Mol	Chain	Res	Type
1	C	52	ASN
1	C	101	ASN
1	C	180	ASN
2	D	17	GLN
2	D	26	GLN
2	D	66	HIS
2	D	86	GLN
2	E	26	GLN
2	E	66	HIS
2	F	17	GLN
2	F	26	GLN
2	F	32	ASN
2	F	52	ASN
2	F	66	HIS
2	F	77	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SCH	B	25[A]	-	6,7,8	0.47	0	4,7,9	0.32	0
1	SCH	C	25[B]	-	6,7,8	0.58	0	4,7,9	0.33	0
1	SCH	C	25[A]	-	6,7,8	0.53	0	4,7,9	0.39	0
1	SCH	B	25[B]	-	6,7,8	0.38	0	4,7,9	0.95	0
1	SCH	A	25	1	6,7,8	0.36	0	4,7,9	0.62	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
1	SCH	B	25[A]	-	-	0/2/6/8	-
1	SCH	C	25[B]	-	-	0/2/6/8	-
1	SCH	C	25[A]	-	-	0/2/6/8	-
1	SCH	B	25[B]	-	-	0/2/6/8	-
1	SCH	A	25	1	-	0/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	25[A]	SCH	10	0
1	C	25[B]	SCH	15	0
1	C	25[A]	SCH	4	0
1	B	25[B]	SCH	6	0
1	A	25	SCH	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [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	217/220 (98%)	-1.49	0 100 100	8, 13, 26, 44	9 (4%)
1	B	218/220 (99%)	-1.46	0 100 100	8, 14, 27, 47	6 (2%)
1	C	218/220 (99%)	-1.48	0 100 100	8, 13, 26, 41	7 (3%)
2	D	98/98 (100%)	-1.47	0 100 100	10, 17, 32, 37	3 (3%)
2	E	98/98 (100%)	-1.45	0 100 100	10, 16, 33, 43	0
2	F	98/98 (100%)	-1.47	0 100 100	10, 16, 35, 41	1 (1%)
All	All	947/954 (99%)	-1.47	0 100 100	8, 14, 28, 47	26 (2%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	SCH	A	25	8/9	0.99	0.03	6,9,12,16	0
1	SCH	B	25[A]	8/9	1.00	0.03	8,11,19,22	4
1	SCH	B	25[B]	8/9	1.00	0.03	8,11,19,22	4
1	SCH	C	25[A]	8/9	1.00	0.02	8,9,13,18	4
1	SCH	C	25[B]	8/9	1.00	0.02	8,9,13,18	4

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.