



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:25 AM UTC

PDB ID : 5L8S / pdb_00005l8s
Title : The crystal structure of a cold-adapted acylaminoacyl peptidase reveals a novel quaternary architecture based on the arm-exchange mechanism
Authors : Brocca, S.; Ferrari, C.; Barbiroli, A.; Pesce, A.; Lotti, M.; Nardini, M.
Deposited on : 2016-06-08
Resolution : 2.50 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

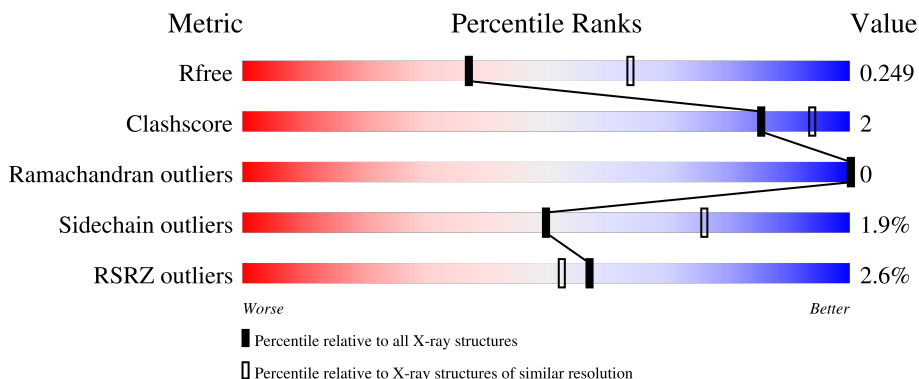
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	604	2% 94% 6%
1	B	604	4% 92% 8%
1	C	604	3% 93% 7%
1	D	604	2% 94% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20067 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 Amino acyl peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	2	0
			4893	3139	800	934	20			
1	B	604	Total	C	N	O	S	0	2	0
			4893	3139	800	934	20			
1	C	604	Total	C	N	O	S	0	1	0
			4887	3135	800	932	20			
1	D	604	Total	C	N	O	S	0	2	0
			4893	3139	800	934	20			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	597	LEU	-	expression tag	UNP E1VFE0
A	598	GLU	-	expression tag	UNP E1VFE0
A	599	HIS	-	expression tag	UNP E1VFE0
A	600	HIS	-	expression tag	UNP E1VFE0
A	601	HIS	-	expression tag	UNP E1VFE0
A	602	HIS	-	expression tag	UNP E1VFE0
A	603	HIS	-	expression tag	UNP E1VFE0
A	604	HIS	-	expression tag	UNP E1VFE0
B	597	LEU	-	expression tag	UNP E1VFE0
B	598	GLU	-	expression tag	UNP E1VFE0
B	599	HIS	-	expression tag	UNP E1VFE0
B	600	HIS	-	expression tag	UNP E1VFE0
B	601	HIS	-	expression tag	UNP E1VFE0
B	602	HIS	-	expression tag	UNP E1VFE0
B	603	HIS	-	expression tag	UNP E1VFE0
B	604	HIS	-	expression tag	UNP E1VFE0
C	597	LEU	-	expression tag	UNP E1VFE0
C	598	GLU	-	expression tag	UNP E1VFE0
C	599	HIS	-	expression tag	UNP E1VFE0
C	600	HIS	-	expression tag	UNP E1VFE0
C	601	HIS	-	expression tag	UNP E1VFE0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	602	HIS	-	expression tag	UNP E1VFE0
C	603	HIS	-	expression tag	UNP E1VFE0
C	604	HIS	-	expression tag	UNP E1VFE0
D	597	LEU	-	expression tag	UNP E1VFE0
D	598	GLU	-	expression tag	UNP E1VFE0
D	599	HIS	-	expression tag	UNP E1VFE0
D	600	HIS	-	expression tag	UNP E1VFE0
D	601	HIS	-	expression tag	UNP E1VFE0
D	602	HIS	-	expression tag	UNP E1VFE0
D	603	HIS	-	expression tag	UNP E1VFE0
D	604	HIS	-	expression tag	UNP E1VFE0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

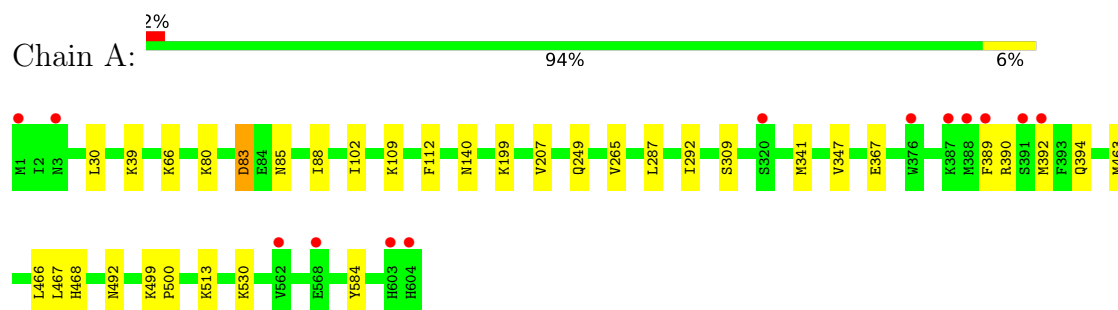
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total 181	O 181	0	4
3	B	107	Total 107	O 107	0	0
3	C	105	Total 106	O 106	0	1
3	D	87	Total 87	O 87	0	0

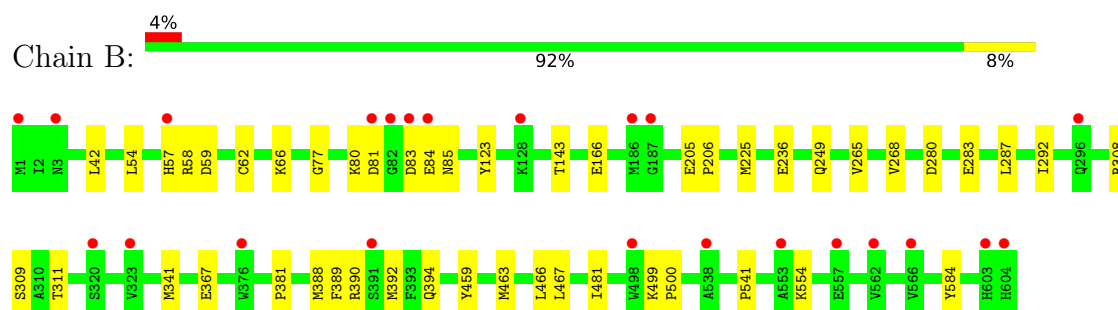
3 Residue-property plots [i](#)

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.

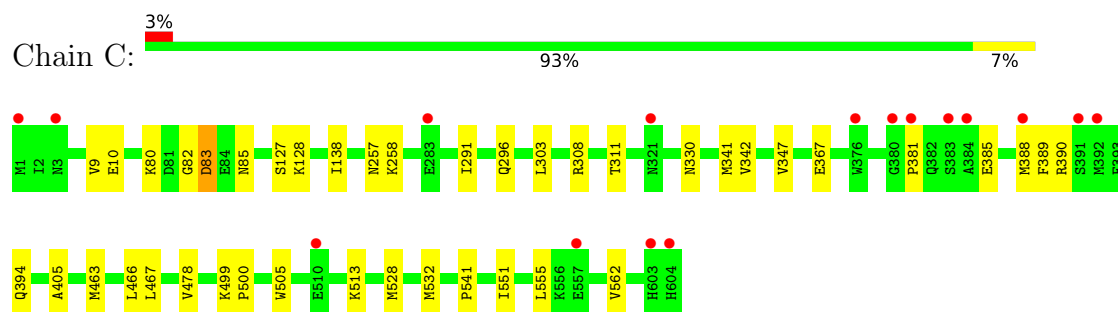
• Molecule 1: Amino acyl peptidase



• Molecule 1: Amino acyl peptidase

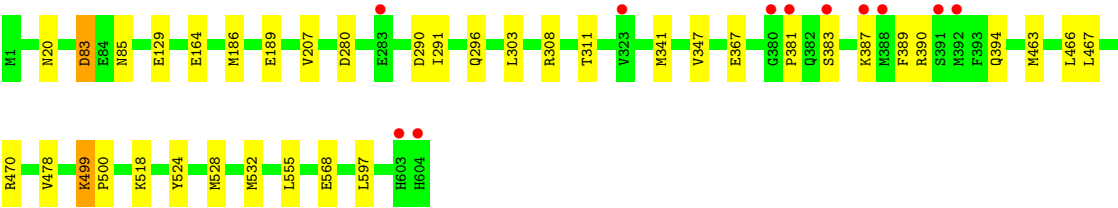


• Molecule 1: Amino acyl peptidase



• Molecule 1: Amino acyl peptidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.08Å 151.10Å 191.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.48 – 2.50 63.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.48-2.50) 99.9 (63.48-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.02 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.212 , 0.248 0.214 , 0.249	Depositor DCC
R_{free} test set	7433 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.056 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20067	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 44.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4490e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.63	0/5030	0.80	0/6815
1	B	0.63	0/5030	0.82	2/6815 (0.0%)
1	C	0.65	0/5021	0.83	3/6803 (0.0%)
1	D	0.66	0/5030	0.80	0/6815
All	All	0.64	0/20111	0.81	5/27248 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	ILE	N-CA-C	8.70	119.20	106.85
1	B	481	ILE	CB-CA-C	-7.01	102.42	111.53
1	C	82	GLY	CA-C-N	5.32	128.81	120.82
1	C	82	GLY	C-N-CA	5.32	128.81	120.82
1	C	342	VAL	N-CA-C	5.14	115.71	108.36

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	4893	0	4702	19	0
1	B	4893	0	4702	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4887	0	4696	22	0
1	D	4893	0	4702	18	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	181	0	0	0	0
3	B	107	0	0	0	0
3	C	106	0	0	0	0
3	D	87	0	0	0	0
All	All	20067	0	18802	85	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 2.

All (85) 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:84:GLU:HG3	1:B:541:PRO:HG3	1.48	0.93
1:B:80:LYS:O	1:B:83:ASP:HB2	1.82	0.79
1:B:463:MET:HE1	1:B:466:LEU:HD23	1.65	0.78
1:B:84:GLU:HG3	1:B:541:PRO:CG	2.14	0.77
1:B:463:MET:HE2	1:B:467:LEU:HG	1.66	0.76
1:D:463:MET:HE2	1:D:467:LEU:HG	1.66	0.76
1:B:341:MET:HE3	1:B:394:GLN:HG3	1.76	0.67
1:B:463:MET:HA	1:B:463:MET:HE3	1.78	0.66
1:C:341:MET:HE3	1:C:394:GLN:HG3	1.77	0.65
1:C:463:MET:HE2	1:C:467:LEU:HG	1.80	0.63
1:D:341:MET:HE3	1:D:394:GLN:HG3	1.80	0.61
1:C:463:MET:HE1	1:C:466:LEU:HD23	1.82	0.61
1:D:291:ILE:HD13	1:D:387:LYS:O	2.00	0.61
1:B:84:GLU:CG	1:B:541:PRO:HG3	2.26	0.60
1:A:249:GLN:HG3	1:A:265:VAL:HG23	1.86	0.58
1:A:463:MET:HE3	1:A:463:MET:HA	1.85	0.58
1:B:463:MET:HE3	1:B:466:LEU:HB3	1.86	0.57
1:C:463:MET:HA	1:C:463:MET:HE3	1.87	0.56
1:A:80:LYS:O	1:A:83:ASP:HB2	2.05	0.56
1:A:83:ASP:HB3	1:A:85:ASN:H	1.70	0.56
1:B:309:SER:O	1:B:389:PHE:HB2	2.05	0.56
1:A:463:MET:HE2	1:A:467:LEU:HG	1.90	0.54
1:D:518:LYS:O	1:D:524:TYR:OH	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:MET:HE1	1:C:551:ILE:HD11	1.90	0.52
1:A:463:MET:HE3	1:A:466:LEU:HB3	1.90	0.52
1:A:309:SER:O	1:A:389:PHE:N	2.43	0.51
1:C:296[B]:GLN:HE21	1:C:296[B]:GLN:HA	1.75	0.51
1:B:83:ASP:C	1:B:85:ASN:H	2.18	0.51
1:C:381:PRO:HD2	1:C:505:TRP:HZ2	1.74	0.51
1:D:83:ASP:HB3	1:D:85:ASN:H	1.76	0.50
1:A:463:MET:HE1	1:A:466:LEU:HD23	1.92	0.50
1:C:291:ILE:HG13	1:C:388:MET:HB3	1.94	0.50
1:D:478:VAL:HB	1:D:532:MET:HE3	1.94	0.49
1:D:463:MET:HE3	1:D:466:LEU:HB3	1.93	0.49
1:B:392:MET:HE2	1:B:584:TYR:HE1	1.78	0.49
1:C:555:LEU:HB3	1:C:562:VAL:HG21	1.94	0.49
1:B:249:GLN:HG2	1:B:265:VAL:HG23	1.95	0.48
1:B:311:THR:HA	1:B:341:MET:HE2	1.96	0.48
1:C:528:MET:HE2	1:C:555:LEU:HD21	1.95	0.47
1:B:499:LYS:HB2	1:B:500:PRO:HD3	1.95	0.47
1:A:66:LYS:HG3	1:A:112:PHE:CZ	2.50	0.47
1:B:80:LYS:O	1:B:81:ASP:C	2.57	0.47
1:C:381:PRO:HD2	1:C:505:TRP:CZ2	2.49	0.47
1:D:463:MET:HE1	1:D:466:LEU:HD23	1.96	0.47
1:C:83:ASP:HB3	1:C:85:ASN:H	1.80	0.46
1:A:249:GLN:HG3	1:A:265:VAL:CG2	2.46	0.45
1:A:287:LEU:HD13	1:A:292:ILE:HD11	1.98	0.45
1:C:127:SER:O	1:C:128:LYS:C	2.60	0.45
1:A:30:LEU:C	1:A:30:LEU:HD23	2.41	0.44
1:D:290:ASP:C	1:D:291:ILE:HD12	2.42	0.44
1:A:468:HIS:HE2	1:A:530:LYS:H	1.65	0.44
1:A:88:ILE:HB	1:A:102:ILE:HB	1.99	0.44
1:B:58:ARG:O	1:B:59:ASP:HB2	2.17	0.43
1:C:385:GLU:HG2	1:C:405:ALA:HB1	2.00	0.43
1:A:392:MET:HE2	1:A:584:TYR:HE1	1.84	0.43
1:B:205:GLU:N	1:B:206:PRO:CD	2.82	0.43
1:A:140:ASN:C	1:A:140:ASN:OD1	2.61	0.43
1:A:341:MET:HE3	1:A:394:GLN:HG3	2.01	0.43
1:D:528:MET:HE2	1:D:555:LEU:HD21	2.00	0.43
1:B:287:LEU:HD13	1:B:292:ILE:HD11	2.01	0.42
1:D:280:ASP:O	1:D:280:ASP:CG	2.60	0.42
1:D:311:THR:HA	1:D:341:MET:HE2	2.00	0.42
1:B:280:ASP:CG	1:B:280:ASP:O	2.62	0.42
1:B:381:PRO:HB3	1:B:459:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296[B]:GLN:HE21	1:D:296[B]:GLN:HA	1.84	0.42
1:D:499:LYS:HB2	1:D:500:PRO:HD3	2.02	0.42
1:B:62:CYS:HA	1:B:77:GLY:O	2.19	0.42
1:C:83:ASP:O	1:C:541:PRO:HG3	2.19	0.42
1:C:478:VAL:HB	1:C:532:MET:HE3	2.01	0.42
1:C:311:THR:HA	1:C:341:MET:HE2	2.01	0.42
1:D:186:MET:O	1:D:189:GLU:HG3	2.20	0.42
1:C:308:ARG:HD2	1:C:389:PHE:N	2.36	0.41
1:D:308:ARG:HG3	1:D:389:PHE:H	1.85	0.41
1:A:499:LYS:HB2	1:A:500:PRO:HD3	2.01	0.41
1:C:257:ASN:O	1:C:258:LYS:C	2.62	0.41
1:B:123:TYR:OH	1:B:166:GLU:OE1	2.36	0.41
1:C:499:LYS:HB2	1:C:500:PRO:HD3	2.02	0.41
1:D:470:ARG:HD2	1:D:524:TYR:CZ	2.56	0.41
1:C:80:LYS:O	1:C:83:ASP:HB2	2.20	0.41
1:B:54:LEU:HD21	1:B:57:HIS:HB2	2.03	0.41
1:B:308:ARG:NH2	1:B:388:MET:HE2	2.36	0.40
1:C:341:MET:CE	1:C:389:PHE:HE1	2.34	0.40
1:D:381:PRO:C	1:D:383:SER:H	2.29	0.40
1:B:225:MET:HE3	1:B:225:MET:HB3	2.01	0.40
1:A:249:GLN:CG	1:A:265:VAL:HG23	2.50	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	604/604 (100%)	575 (95%)	29 (5%)	0	100	100
1	B	604/604 (100%)	584 (97%)	20 (3%)	0	100	100
1	C	603/604 (100%)	578 (96%)	25 (4%)	0	100	100
1	D	604/604 (100%)	577 (96%)	27 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2415/2416 (100%)	2314 (96%)	101 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	533/531 (100%)	523 (98%)	10 (2%)	50	76
1	B	533/531 (100%)	523 (98%)	10 (2%)	50	76
1	C	532/531 (100%)	522 (98%)	10 (2%)	50	76
1	D	533/531 (100%)	521 (98%)	12 (2%)	44	72
All	All	2131/2124 (100%)	2089 (98%)	42 (2%)	50	75

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	83	ASP
1	A	109	LYS
1	A	199	LYS
1	A	207	VAL
1	A	347	VAL
1	A	367	GLU
1	A	390	ARG
1	A	492	ASN
1	A	513	LYS
1	B	42	LEU
1	B	66	LYS
1	B	143	THR
1	B	236[A]	GLU
1	B	236[B]	GLU
1	B	268	VAL
1	B	283	GLU

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Mol	Chain	Res	Type
1	B	367	GLU
1	B	390	ARG
1	B	554	LYS
1	C	9	VAL
1	C	10	GLU
1	C	83	ASP
1	C	138	ILE
1	C	303	LEU
1	C	330	ASN
1	C	347	VAL
1	C	367	GLU
1	C	390	ARG
1	C	513	LYS
1	D	20	ASN
1	D	83	ASP
1	D	129	GLU
1	D	164	GLU
1	D	207	VAL
1	D	303	LEU
1	D	347	VAL
1	D	367	GLU
1	D	390	ARG
1	D	499	LYS
1	D	568	GLU
1	D	597	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	249	GLN
1	B	33	ASN
1	B	93	ASN
1	B	471	HIS
1	B	599	HIS
1	C	3	ASN
1	C	33	ASN
1	C	330	ASN
1	C	331	ASN
1	C	471	HIS
1	C	599	HIS
1	D	3	ASN

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Mol	Chain	Res	Type
1	D	33	ASN
1	D	93	ASN
1	D	99	HIS
1	D	327	GLN
1	D	471	HIS
1	D	595	GLN

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	701	-	4,4,4	0.50	0	6,6,6	0.13	0
2	SO4	D	701	-	4,4,4	0.63	0	6,6,6	0.20	0
2	SO4	B	701	-	4,4,4	0.66	0	6,6,6	0.21	0
2	SO4	A	701	-	4,4,4	0.52	0	6,6,6	0.26	0

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.

No monomer is involved in short contacts.

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	604/604 (100%)	0.07	13 (2%) 62 58	21, 41, 65, 120	2 (0%)
1	B	604/604 (100%)	0.14	23 (3%) 44 39	22, 43, 67, 128	2 (0%)
1	C	604/604 (100%)	0.09	16 (2%) 57 52	20, 43, 65, 117	1 (0%)
1	D	604/604 (100%)	0.03	11 (1%) 67 64	19, 41, 65, 115	2 (0%)
All	All	2416/2416 (100%)	0.08	63 (2%) 57 52	19, 42, 66, 128	7 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	380	GLY	6.2
1	A	604	HIS	5.2
1	D	380	GLY	5.0
1	B	604	HIS	4.5
1	D	604	HIS	4.4
1	C	604	HIS	4.3
1	A	1	MET	3.8
1	B	83	ASP	3.8
1	D	388	MET	3.6
1	B	1	MET	3.5
1	B	603	HIS	3.3
1	D	383	SER	3.3
1	C	1	MET	3.1
1	C	388	MET	3.1
1	B	553	ALA	3.0
1	D	392	MET	3.0
1	D	603	HIS	2.9
1	C	381	PRO	2.9
1	A	392	MET	2.9
1	A	603	HIS	2.9
1	A	391	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	82	GLY	2.7
1	A	376	TRP	2.7
1	A	388	MET	2.6
1	C	392	MET	2.6
1	D	323	VAL	2.6
1	B	538	ALA	2.6
1	B	186	MET	2.5
1	B	376	TRP	2.5
1	C	510	GLU	2.5
1	B	562	VAL	2.5
1	D	381	PRO	2.5
1	C	3	ASN	2.4
1	B	391	SER	2.4
1	B	84	GLU	2.4
1	D	387	LYS	2.4
1	B	557	GLU	2.4
1	D	391	SER	2.3
1	B	3	ASN	2.3
1	B	187	GLY	2.3
1	A	320	SER	2.3
1	A	387	LYS	2.3
1	B	320	SER	2.2
1	A	568	GLU	2.2
1	A	562	VAL	2.2
1	B	57	HIS	2.2
1	B	128	LYS	2.2
1	C	376	TRP	2.2
1	A	389	PHE	2.2
1	B	323	VAL	2.2
1	C	384	ALA	2.2
1	B	81	ASP	2.2
1	A	3	ASN	2.1
1	C	557	GLU	2.1
1	D	283	GLU	2.1
1	C	383	SER	2.1
1	B	296[A]	GLN	2.1
1	C	321	ASN	2.1
1	C	391	SER	2.1
1	C	603	HIS	2.1
1	B	566	VAL	2.0
1	C	283	GLU	2.0
1	B	498	TRP	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SO4	A	701	5/5	0.81	0.16	70,76,78,85	0
2	SO4	B	701	5/5	0.83	0.15	58,61,65,73	0
2	SO4	D	701	5/5	0.83	0.14	67,69,77,85	0
2	SO4	C	701	5/5	0.90	0.13	75,75,84,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.