Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 11:17 AM EDT

PDB ID	:	5N7N
Title	:	CRYSTAL STRUCTURE OF CATHEPSIN D ZYMOGEN FROM THE TICK IXODES RICINUS (IRCD1)
Authors	:	Brynda, J.; Hanova, I.; Hobizalova, R.; Mares, M.
Deposited on	:	2017-02-21
Resolution	:	2.30 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:

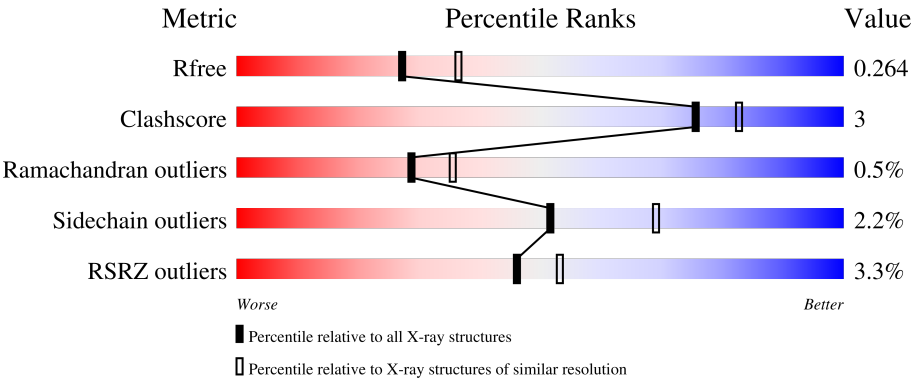
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	367	7% 89% 8%
1	B	367	2% 91% 7%
1	C	367	2% 88% 10%
1	D	367	3% 90% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11207 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 Putative cathepsin d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2735	1750	444	530	11			
1	B	361	Total	C	N	O	S	0	1	0
			2757	1765	448	533	11			
1	C	361	Total	C	N	O	S	0	0	0
			2755	1762	449	533	11			
1	D	360	Total	C	N	O	S	0	0	0
			2717	1741	439	526	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	VAL	GLU	conflict	UNP V5HCK7
A	182	LEU	ARG	conflict	UNP V5HCK7
A	249	ASN	ASP	conflict	UNP V5HCK7
A	362	HIS	-	expression tag	UNP V5HCK7
A	363	HIS	-	expression tag	UNP V5HCK7
A	364	HIS	-	expression tag	UNP V5HCK7
A	365	HIS	-	expression tag	UNP V5HCK7
A	366	HIS	-	expression tag	UNP V5HCK7
A	367	HIS	-	expression tag	UNP V5HCK7
B	39	VAL	GLU	conflict	UNP V5HCK7
B	182	LEU	ARG	conflict	UNP V5HCK7
B	249	ASN	ASP	conflict	UNP V5HCK7
B	362	HIS	-	expression tag	UNP V5HCK7
B	363	HIS	-	expression tag	UNP V5HCK7
B	364	HIS	-	expression tag	UNP V5HCK7
B	365	HIS	-	expression tag	UNP V5HCK7
B	366	HIS	-	expression tag	UNP V5HCK7
B	367	HIS	-	expression tag	UNP V5HCK7
C	39	VAL	GLU	conflict	UNP V5HCK7
C	182	LEU	ARG	conflict	UNP V5HCK7
C	249	ASN	ASP	conflict	UNP V5HCK7

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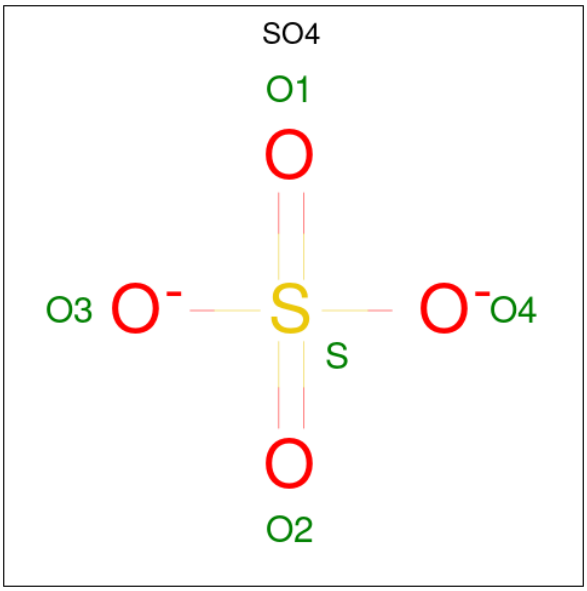
Chain	Residue	Modelled	Actual	Comment	Reference
C	362	HIS	-	expression tag	UNP V5HCK7
C	363	HIS	-	expression tag	UNP V5HCK7
C	364	HIS	-	expression tag	UNP V5HCK7
C	365	HIS	-	expression tag	UNP V5HCK7
C	366	HIS	-	expression tag	UNP V5HCK7
C	367	HIS	-	expression tag	UNP V5HCK7
D	39	VAL	GLU	conflict	UNP V5HCK7
D	182	LEU	ARG	conflict	UNP V5HCK7
D	249	ASN	ASP	conflict	UNP V5HCK7
D	362	HIS	-	expression tag	UNP V5HCK7
D	363	HIS	-	expression tag	UNP V5HCK7
D	364	HIS	-	expression tag	UNP V5HCK7
D	365	HIS	-	expression tag	UNP V5HCK7
D	366	HIS	-	expression tag	UNP V5HCK7
D	367	HIS	-	expression tag	UNP V5HCK7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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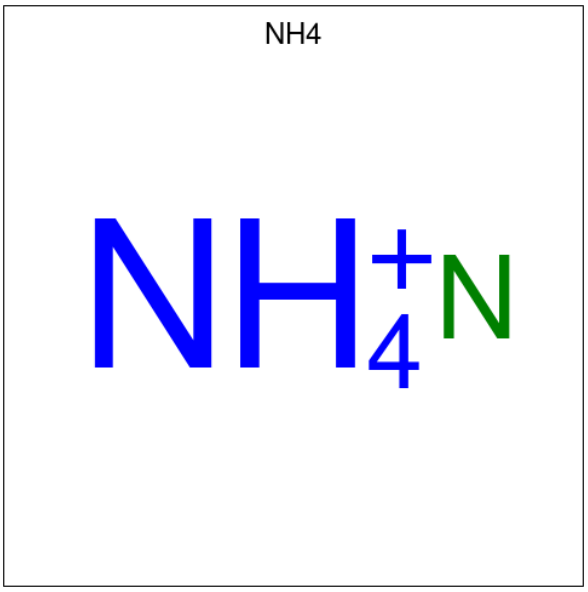
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0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

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 1 1	0	0
3	B	1	Total N 1 1	0	0
3	C	1	Total N 1 1	0	0
3	D	1	Total N 1 1	0	0

- Molecule 4 is water.

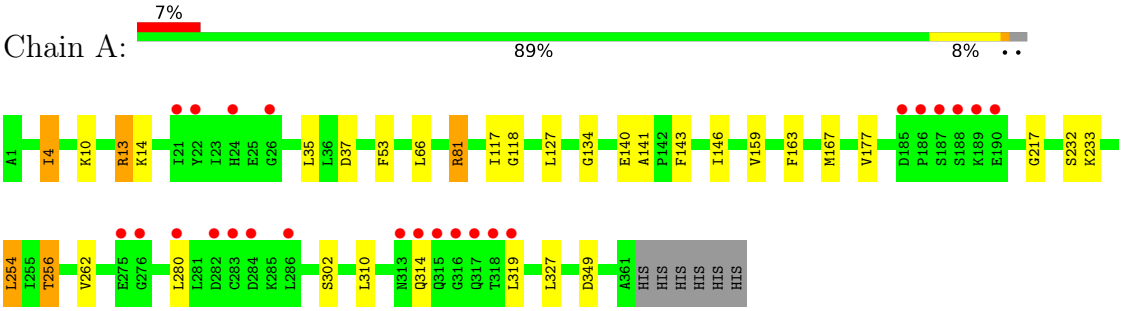
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	52	Total O 53 53	0	1
4	C	37	Total O 37 37	0	0
4	D	28	Total O 29 29	0	1

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.

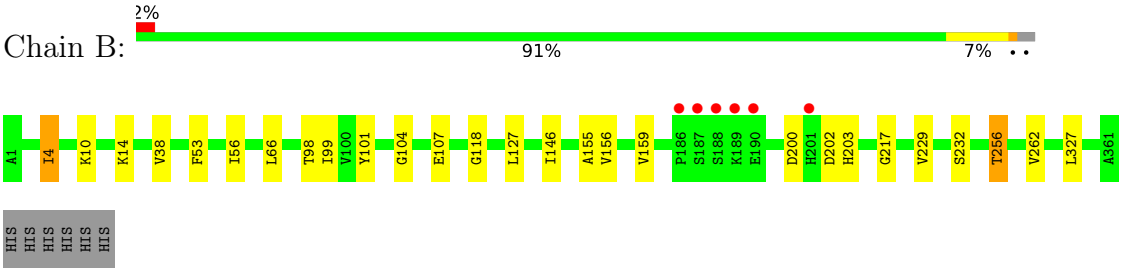
• Molecule 1: Putative cathepsin d

Chain A:



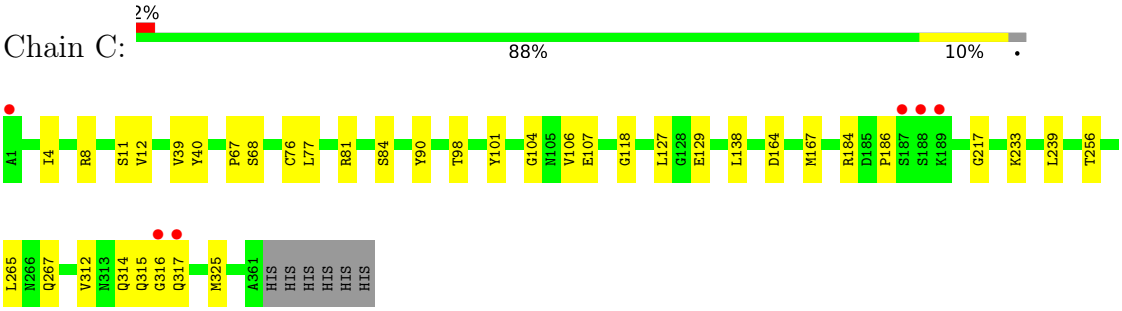
• Molecule 1: Putative cathepsin d

Chain B:



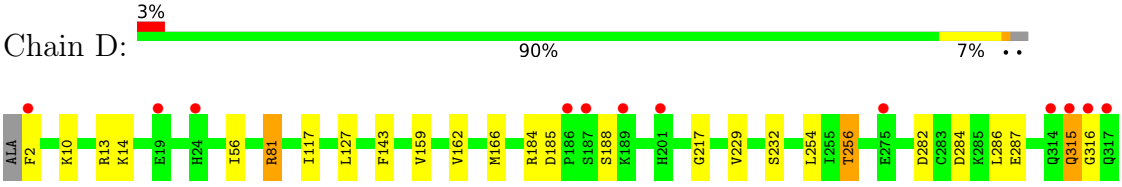
• Molecule 1: Putative cathepsin d

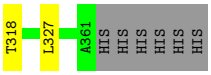
Chain C:



• Molecule 1: Putative cathepsin d

Chain D:




T318
L327
A361
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.32Å 94.98Å 106.17Å 90.00° 99.28° 90.00°	Depositor
Resolution (Å)	45.87 – 2.30 45.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.87-2.30) 99.8 (45.87-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.220 , 0.260 0.222 , 0.264	Depositor DCC
R_{free} test set	4145 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11207	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NH4, 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	0.46	0/2803	0.71	3/3815 (0.1%)
1	B	0.54	0/2828	0.74	0/3846
1	C	0.50	0/2823	0.72	1/3838 (0.0%)
1	D	0.48	0/2785	0.72	5/3793 (0.1%)
All	All	0.50	0/11239	0.72	9/15292 (0.1%)

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	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	81	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	D	13	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	D	13	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	81	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	13	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	13	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	D	184	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	184	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	D	81	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2	PHE	Peptide
1	D	286	LEU	Peptide

5.2 Too-close contacts (i)

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	2735	0	2622	14	1
1	B	2757	0	2670	21	0
1	C	2755	0	2668	22	1
1	D	2717	0	2589	12	1
2	A	15	0	0	0	0
2	B	30	0	0	0	0
2	C	25	0	0	0	0
2	D	20	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	30	0	0	2	0
4	B	53	0	0	6	0
4	C	37	0	0	0	0
4	D	29	0	0	0	0
All	All	11207	0	10549	67	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 3.

All (67) 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:D:315:GLN:CB	1:D:316:GLY:HA3	2.12	0.80
1:C:315:GLN:CB	1:C:316:GLY:HA3	2.12	0.78
1:C:8:ARG:NH2	1:C:186:PRO:HA	2.07	0.69
1:C:8:ARG:HH21	1:C:186:PRO:HA	1.59	0.68
1:C:77:LEU:HB3	1:D:229:VAL:HG13	1.75	0.68
1:B:4:ILE:HD11	1:B:118:GLY:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:THR:HG23	1:B:327:LEU:HB3	1.81	0.62
1:D:256:THR:HG23	1:D:327:LEU:HB3	1.82	0.60
1:B:99[A]:ILE:HD11	4:B:552:HOH:O	2.04	0.58
1:D:10:LYS:HG3	1:D:14:LYS:HD3	1.85	0.58
1:B:98:THR:HG23	1:B:107:GLU:HG2	1.86	0.57
1:C:76:CYS:O	1:C:81:ARG:HD2	2.04	0.57
1:A:256:THR:HG23	1:A:327:LEU:HB3	1.88	0.55
1:C:314:GLN:HB3	1:C:317:GLN:HG2	1.89	0.54
1:C:39:VAL:HG12	1:C:40:TYR:CD2	2.43	0.53
1:C:77:LEU:HB3	1:D:229:VAL:CG1	2.38	0.53
1:C:4:ILE:HD11	1:C:118:GLY:N	2.23	0.53
1:C:12:VAL:HG21	1:C:138:LEU:HD23	1.91	0.53
1:B:99[A]:ILE:HD13	1:B:101:TYR:HE1	1.73	0.53
1:B:203:HIS:CE1	4:B:501:HOH:O	2.63	0.52
1:D:256:THR:CG2	1:D:327:LEU:HB3	2.40	0.51
1:B:38:VAL:HG21	1:B:56:ILE:HD11	1.91	0.51
1:A:256:THR:HG22	4:A:509:HOH:O	2.11	0.50
1:B:200:ASP:OD1	1:B:202:ASP:HB2	2.12	0.50
1:B:38:VAL:HG21	1:B:56:ILE:CD1	2.41	0.50
1:A:10:LYS:HG3	1:A:14:LYS:HD3	1.95	0.48
1:C:84:SER:HB2	1:C:90:TYR:CD1	2.49	0.48
1:C:164:ASP:HA	1:C:167:MET:HE2	1.96	0.48
1:B:4:ILE:HD11	1:B:118:GLY:CA	2.43	0.47
1:A:254:LEU:HD22	1:A:310:LEU:HD11	1.96	0.47
1:B:203:HIS:HE1	4:B:501:HOH:O	1.97	0.47
1:C:315:GLN:CB	1:C:316:GLY:CA	2.90	0.47
1:B:101:TYR:HB2	1:B:104:GLY:O	2.15	0.46
1:B:56:ILE:HD12	1:B:146:ILE:HD13	1.97	0.46
1:A:256:THR:CG2	4:A:509:HOH:O	2.63	0.46
1:D:185:ASP:HB3	1:D:188:SER:HB3	1.98	0.46
1:A:35:LEU:HD21	1:A:146:ILE:HD11	1.98	0.46
1:C:98:THR:HG23	1:C:107:GLU:HG2	1.97	0.46
1:C:39:VAL:HG12	1:C:40:TYR:CE2	2.52	0.44
1:A:134:GLY:O	3:A:404:NH4:N	2.51	0.44
1:C:256:THR:HA	1:C:325:MET:O	2.18	0.44
1:A:53:PHE:CD2	1:A:66:LEU:HD22	2.53	0.44
1:A:280:LEU:HD22	1:A:319:LEU:HD21	1.99	0.43
1:C:164:ASP:HA	1:C:167:MET:CE	2.49	0.43
1:D:282:ASP:OD1	1:D:284:ASP:HB2	2.17	0.43
1:D:315:GLN:CB	1:D:316:GLY:CA	2.93	0.43
1:A:13:ARG:HD2	1:A:37:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:PHE:CD1	1:B:66:LEU:HD22	2.54	0.43
1:B:256:THR:CG2	4:B:528:HOH:O	2.67	0.43
1:D:117:ILE:HD12	1:D:166:MET:HE3	2.01	0.43
1:D:117:ILE:CD1	1:D:162:VAL:HG11	2.49	0.43
1:D:56:ILE:HD11	1:D:143:PHE:CG	2.54	0.42
1:A:141:ALA:HB1	1:A:143:PHE:CE2	2.55	0.42
1:C:67:PRO:HB2	1:C:81:ARG:HG3	2.01	0.42
1:A:177:VAL:HG12	1:A:349:ASP:HA	2.02	0.42
1:B:155:ALA:HB1	1:B:159:VAL:HG22	2.02	0.42
1:C:101:TYR:HB2	1:C:104:GLY:O	2.20	0.42
1:A:163:PHE:O	1:A:167:MET:HG3	2.20	0.41
1:C:11:SER:HB3	1:C:39:VAL:HG23	2.02	0.41
1:B:99[A]:ILE:HD13	1:B:99[A]:ILE:HG21	1.80	0.41
1:B:156:VAL:HG23	1:B:159:VAL:HG13	2.03	0.41
1:C:68:SER:HB2	1:C:129:GLU:HB3	2.03	0.41
1:B:99[A]:ILE:CD1	4:B:541:HOH:O	2.68	0.41
1:B:256:THR:HG22	4:B:528:HOH:O	2.21	0.41
1:C:239:LEU:HD11	1:C:265:LEU:HB2	2.03	0.41
1:A:4:ILE:HD11	1:A:118:GLY:N	2.37	0.40
1:B:10:LYS:HG3	1:B:14:LYS:HD3	2.02	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)
1:A:81:ARG:NH2	1:A:233:LYS:O[2_556]	2.10	0.10
1:C:233:LYS:O	1:D:81:ARG:NH2[1_655]	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	359/367 (98%)	347 (97%)	10 (3%)	2 (1%)	25	31
1	B	360/367 (98%)	352 (98%)	7 (2%)	1 (0%)	41	50
1	C	359/367 (98%)	350 (98%)	8 (2%)	1 (0%)	41	50
1	D	358/367 (98%)	347 (97%)	8 (2%)	3 (1%)	19	23
All	All	1436/1468 (98%)	1396 (97%)	33 (2%)	7 (0%)	29	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	315	GLN
1	A	314	GLN
1	D	287	GLU
1	B	217	GLY
1	A	217	GLY
1	C	217	GLY
1	D	217	GLY

5.3.2 Protein sidechains (i)

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	294/311 (94%)	284 (97%)	10 (3%)	37	51
1	B	300/311 (96%)	294 (98%)	6 (2%)	55	72
1	C	300/311 (96%)	296 (99%)	4 (1%)	69	82
1	D	290/311 (93%)	284 (98%)	6 (2%)	53	70
All	All	1184/1244 (95%)	1158 (98%)	26 (2%)	52	69

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

Mol	Chain	Res	Type
1	A	4	ILE
1	A	117	ILE
1	A	127	LEU
1	A	140	GLU

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Mol	Chain	Res	Type
1	A	159	VAL
1	A	232	SER
1	A	254	LEU
1	A	256	THR
1	A	262	VAL
1	A	302	SER
1	B	4	ILE
1	B	127	LEU
1	B	229	VAL
1	B	232	SER
1	B	256	THR
1	B	262	VAL
1	C	106	VAL
1	C	127	LEU
1	C	267	GLN
1	C	312	VAL
1	D	127	LEU
1	D	159	VAL
1	D	232	SER
1	D	254	LEU
1	D	256	THR
1	D	318	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	203	HIS
1	B	313	ASN
1	D	105	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 4 are modelled with single atom - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	D	403	-	4,4,4	0.32	0	6,6,6	0.42	0
2	SO4	B	402	-	4,4,4	0.36	0	6,6,6	0.31	0
2	SO4	C	402	-	4,4,4	0.40	0	6,6,6	0.12	0
2	SO4	D	404	-	4,4,4	0.39	0	6,6,6	0.21	0
2	SO4	A	403	-	4,4,4	0.39	0	6,6,6	0.24	0
2	SO4	C	406	-	4,4,4	0.66	0	6,6,6	0.34	0
2	SO4	B	405	-	4,4,4	0.33	0	6,6,6	0.49	0
2	SO4	B	403	-	4,4,4	0.43	0	6,6,6	0.21	0
2	SO4	A	402	-	4,4,4	0.42	0	6,6,6	0.28	0
2	SO4	B	404	-	4,4,4	0.42	0	6,6,6	0.29	0
2	SO4	C	401	-	4,4,4	0.38	0	6,6,6	0.19	0
2	SO4	C	403	-	4,4,4	0.30	0	6,6,6	0.32	0
2	SO4	D	401	-	4,4,4	0.32	0	6,6,6	0.35	0
2	SO4	D	402	-	4,4,4	0.34	0	6,6,6	0.35	0
2	SO4	C	404	-	4,4,4	0.42	0	6,6,6	0.23	0
2	SO4	B	407	-	4,4,4	0.50	0	6,6,6	0.72	0
2	SO4	A	401	-	4,4,4	0.31	0	6,6,6	0.30	0
2	SO4	B	401	-	4,4,4	0.33	0	6,6,6	0.15	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 (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, 95^{th} 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	361/367 (98%)	0.21	24 (6%)	18	23	25, 45, 79, 110	0
1	B	361/367 (98%)	-0.19	6 (1%)	70	76	22, 31, 51, 98	1 (0%)
1	C	361/367 (98%)	-0.23	6 (1%)	70	76	22, 33, 58, 92	1 (0%)
1	D	360/367 (98%)	0.07	12 (3%)	46	53	25, 42, 73, 103	1 (0%)
All	All	1443/1468 (98%)	-0.03	48 (3%)	46	53	22, 37, 70, 110	3 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	GLY	5.9
1	D	317	GLN	5.6
1	C	187	SER	5.4
1	D	187	SER	5.3
1	D	315	GLN	5.2
1	A	189	LYS	5.0
1	A	284	ASP	4.7
1	B	187	SER	4.7
1	A	186	PRO	4.6
1	A	318	THR	4.6
1	A	187	SER	4.4
1	D	189	LYS	4.4
1	A	314	GLN	4.1
1	B	188	SER	4.0
1	C	317	GLN	4.0
1	D	316	GLY	3.6
1	B	189	LYS	3.6
1	A	319	LEU	3.5
1	C	316	GLY	3.4
1	D	275	GLU	3.3
1	A	185	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	190	GLU	3.1
1	D	314	GLN	3.1
1	A	276	GLY	3.1
1	A	280	LEU	3.1
1	C	189	LYS	3.0
1	A	315	GLN	2.9
1	D	24	HIS	2.9
1	C	1	ALA	2.9
1	D	186	PRO	2.8
1	A	188	SER	2.8
1	A	317	GLN	2.8
1	A	275	GLU	2.7
1	B	201	HIS	2.7
1	A	283	CYS	2.7
1	B	190	GLU	2.7
1	B	186	PRO	2.5
1	A	22	TYR	2.4
1	D	19	GLU	2.4
1	D	2	PHE	2.4
1	A	26	GLY	2.3
1	D	201	HIS	2.3
1	A	286	LEU	2.3
1	A	313	ASN	2.3
1	A	24	HIS	2.3
1	A	21	ILE	2.1
1	C	188	SER	2.1
1	A	282	ASP	2.1

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, 95^{th} 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
2	SO4	B	404	5/5	0.70	0.23	79,83,96,96	0
2	SO4	D	402	5/5	0.85	0.22	77,82,87,89	0
2	SO4	B	403	5/5	0.87	0.19	68,69,75,76	0
2	SO4	A	402	5/5	0.88	0.21	73,75,82,83	0
2	SO4	C	404	5/5	0.89	0.28	70,73,77,80	0
2	SO4	D	403	5/5	0.89	0.20	81,82,86,87	0
2	SO4	D	404	5/5	0.90	0.15	85,88,91,92	0
2	SO4	C	401	5/5	0.91	0.16	67,72,74,74	0
2	SO4	C	402	5/5	0.92	0.23	67,74,75,79	0
2	SO4	D	401	5/5	0.93	0.14	60,64,68,70	0
2	SO4	B	405	5/5	0.93	0.20	65,68,74,76	0
2	SO4	C	403	5/5	0.93	0.16	63,65,72,76	0
2	SO4	A	403	5/5	0.93	0.11	75,79,85,87	0
2	SO4	B	401	5/5	0.94	0.27	76,78,80,81	0
2	SO4	B	407	5/5	0.94	0.21	45,45,45,46	0
2	SO4	A	401	5/5	0.95	0.11	67,70,74,74	0
2	SO4	B	402	5/5	0.95	0.15	64,64,66,67	0
3	NH4	B	406	1/1	0.95	0.18	21,21,21,21	0
3	NH4	A	404	1/1	0.96	0.16	29,29,29,29	0
3	NH4	D	405	1/1	0.96	0.14	26,26,26,26	0
3	NH4	C	405	1/1	0.98	0.19	17,17,17,17	0
2	SO4	C	406	5/5	0.98	0.16	44,47,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.