Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 03:41 PM JST

PDB ID	:	5ZNZ
Title	:	Structure of mDR3 DD with MBP tag mutant-I387V
Authors	:	Jin, T.; Yin, X.
Deposited on	:	2018-04-12
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

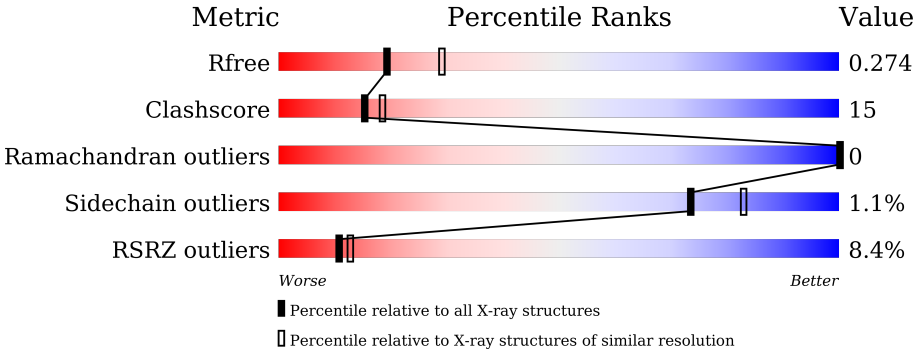
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	464	7% 72% 23% • •
1	B	464	6% 73% 23% • •
1	C	464	12% 68% 25% • •
1	D	464	8% 71% 25% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14119 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 Maltose-binding periplasmic protein,Tumor necrosis factor receptor superfamily, member 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	449	3482	2231	583	657	11	0	0	0
1	B	451	3499	2240	588	660	11	0	0	0
1	C	450	3490	2235	587	657	11	0	0	0
1	D	453	3516	2252	591	662	11	0	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P0AEX9
A	83	ALA	ASP	engineered mutation	UNP P0AEX9
A	84	ALA	LYS	engineered mutation	UNP P0AEX9
A	173	ALA	GLU	engineered mutation	UNP P0AEX9
A	174	ALA	ASN	engineered mutation	UNP P0AEX9
A	240	ALA	LYS	engineered mutation	UNP P0AEX9
A	360	ALA	GLU	engineered mutation	UNP P0AEX9
A	363	ALA	LYS	engineered mutation	UNP P0AEX9
A	364	ALA	ASP	engineered mutation	UNP P0AEX9
A	368	ASN	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	ARG	-	linker	UNP P0AEX9
A	372	ALA	-	linker	UNP P0AEX9
A	373	ALA	-	linker	UNP P0AEX9
A	374	ALA	-	linker	UNP P0AEX9
A	434	VAL	ILE	engineered mutation	UNP B1AWN9
A	457	LEU	-	expression tag	UNP B1AWN9
A	458	GLU	-	expression tag	UNP B1AWN9
A	459	HIS	-	expression tag	UNP B1AWN9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	460	HIS	-	expression tag	UNP B1AWN9
A	461	HIS	-	expression tag	UNP B1AWN9
A	462	HIS	-	expression tag	UNP B1AWN9
A	463	HIS	-	expression tag	UNP B1AWN9
A	464	HIS	-	expression tag	UNP B1AWN9
B	1	MET	-	expression tag	UNP P0AEX9
B	83	ALA	ASP	engineered mutation	UNP P0AEX9
B	84	ALA	LYS	engineered mutation	UNP P0AEX9
B	173	ALA	GLU	engineered mutation	UNP P0AEX9
B	174	ALA	ASN	engineered mutation	UNP P0AEX9
B	240	ALA	LYS	engineered mutation	UNP P0AEX9
B	360	ALA	GLU	engineered mutation	UNP P0AEX9
B	363	ALA	LYS	engineered mutation	UNP P0AEX9
B	364	ALA	ASP	engineered mutation	UNP P0AEX9
B	368	ASN	-	linker	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
B	371	ARG	-	linker	UNP P0AEX9
B	372	ALA	-	linker	UNP P0AEX9
B	373	ALA	-	linker	UNP P0AEX9
B	374	ALA	-	linker	UNP P0AEX9
B	434	VAL	ILE	engineered mutation	UNP B1AWN9
B	457	LEU	-	expression tag	UNP B1AWN9
B	458	GLU	-	expression tag	UNP B1AWN9
B	459	HIS	-	expression tag	UNP B1AWN9
B	460	HIS	-	expression tag	UNP B1AWN9
B	461	HIS	-	expression tag	UNP B1AWN9
B	462	HIS	-	expression tag	UNP B1AWN9
B	463	HIS	-	expression tag	UNP B1AWN9
B	464	HIS	-	expression tag	UNP B1AWN9
C	1	MET	-	expression tag	UNP P0AEX9
C	83	ALA	ASP	engineered mutation	UNP P0AEX9
C	84	ALA	LYS	engineered mutation	UNP P0AEX9
C	173	ALA	GLU	engineered mutation	UNP P0AEX9
C	174	ALA	ASN	engineered mutation	UNP P0AEX9
C	240	ALA	LYS	engineered mutation	UNP P0AEX9
C	360	ALA	GLU	engineered mutation	UNP P0AEX9
C	363	ALA	LYS	engineered mutation	UNP P0AEX9
C	364	ALA	ASP	engineered mutation	UNP P0AEX9
C	368	ASN	-	linker	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9

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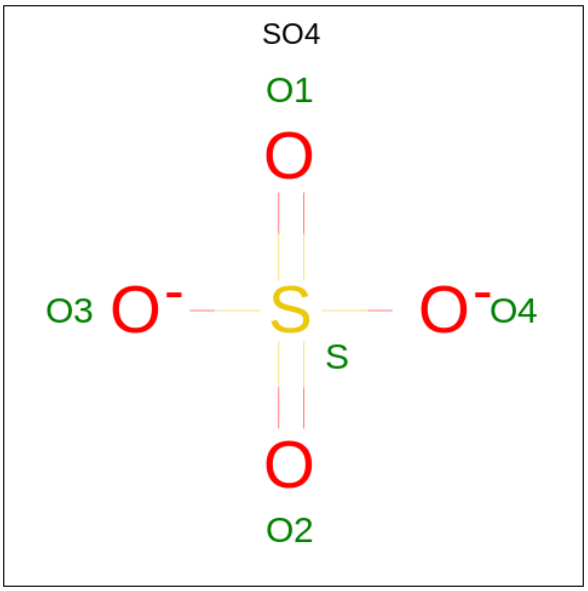
Chain	Residue	Modelled	Actual	Comment	Reference
C	371	ARG	-	linker	UNP P0AEX9
C	372	ALA	-	linker	UNP P0AEX9
C	373	ALA	-	linker	UNP P0AEX9
C	374	ALA	-	linker	UNP P0AEX9
C	434	VAL	ILE	engineered mutation	UNP B1AWN9
C	457	LEU	-	expression tag	UNP B1AWN9
C	458	GLU	-	expression tag	UNP B1AWN9
C	459	HIS	-	expression tag	UNP B1AWN9
C	460	HIS	-	expression tag	UNP B1AWN9
C	461	HIS	-	expression tag	UNP B1AWN9
C	462	HIS	-	expression tag	UNP B1AWN9
C	463	HIS	-	expression tag	UNP B1AWN9
C	464	HIS	-	expression tag	UNP B1AWN9
D	1	MET	-	expression tag	UNP P0AEX9
D	83	ALA	ASP	engineered mutation	UNP P0AEX9
D	84	ALA	LYS	engineered mutation	UNP P0AEX9
D	173	ALA	GLU	engineered mutation	UNP P0AEX9
D	174	ALA	ASN	engineered mutation	UNP P0AEX9
D	240	ALA	LYS	engineered mutation	UNP P0AEX9
D	360	ALA	GLU	engineered mutation	UNP P0AEX9
D	363	ALA	LYS	engineered mutation	UNP P0AEX9
D	364	ALA	ASP	engineered mutation	UNP P0AEX9
D	368	ASN	-	linker	UNP P0AEX9
D	369	ALA	-	linker	UNP P0AEX9
D	370	ALA	-	linker	UNP P0AEX9
D	371	ARG	-	linker	UNP P0AEX9
D	372	ALA	-	linker	UNP P0AEX9
D	373	ALA	-	linker	UNP P0AEX9
D	374	ALA	-	linker	UNP P0AEX9
D	434	VAL	ILE	engineered mutation	UNP B1AWN9
D	457	LEU	-	expression tag	UNP B1AWN9
D	458	GLU	-	expression tag	UNP B1AWN9
D	459	HIS	-	expression tag	UNP B1AWN9
D	460	HIS	-	expression tag	UNP B1AWN9
D	461	HIS	-	expression tag	UNP B1AWN9
D	462	HIS	-	expression tag	UNP B1AWN9
D	463	HIS	-	expression tag	UNP B1AWN9
D	464	HIS	-	expression tag	UNP B1AWN9

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



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

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

- Molecule 3 is water.

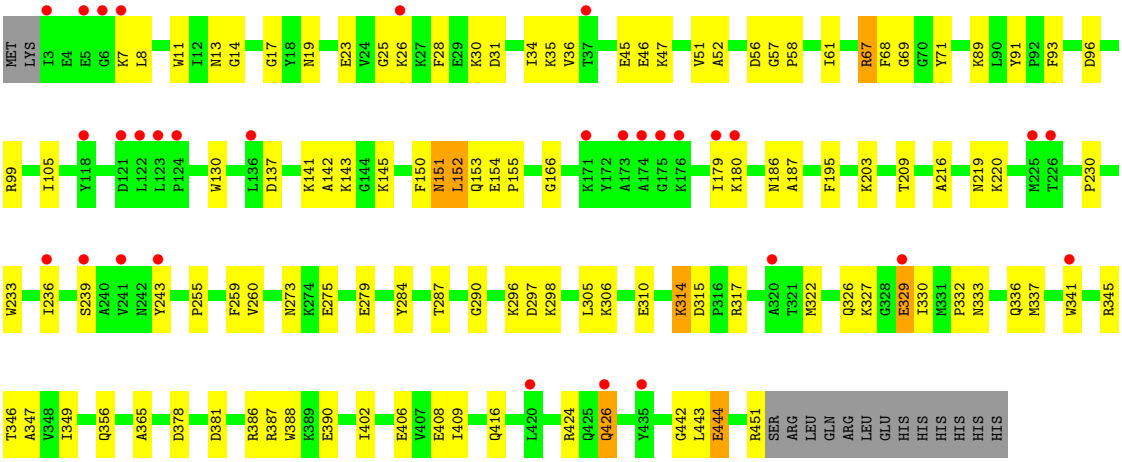
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	2	2	2	0	0

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.

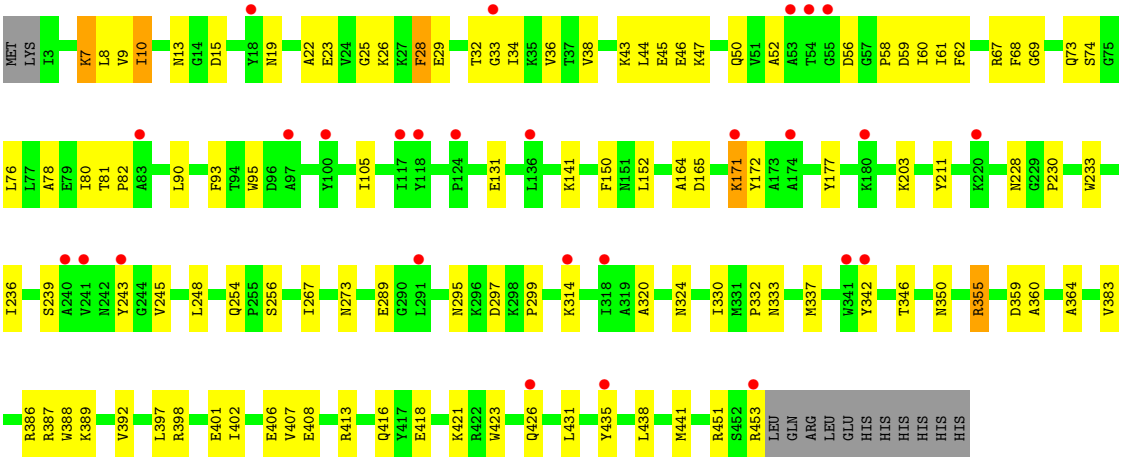
• Molecule 1: Maltose-binding periplasmic protein,Tumor necrosis factor receptor superfamily, member 25

Chain A:



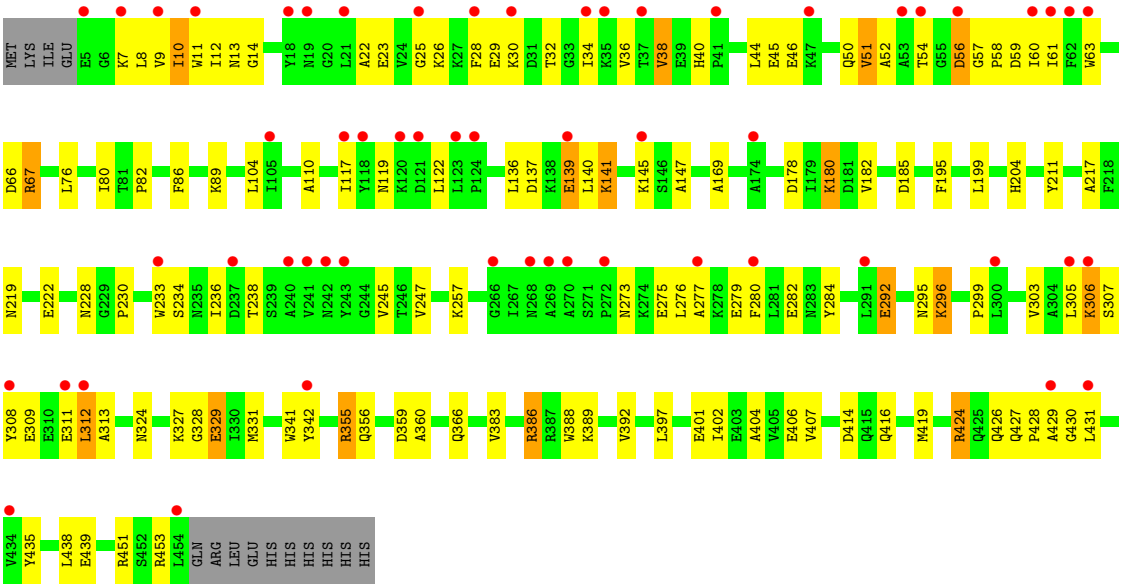
• Molecule 1: Maltose-binding periplasmic protein,Tumor necrosis factor receptor superfamily, member 25

Chain B:



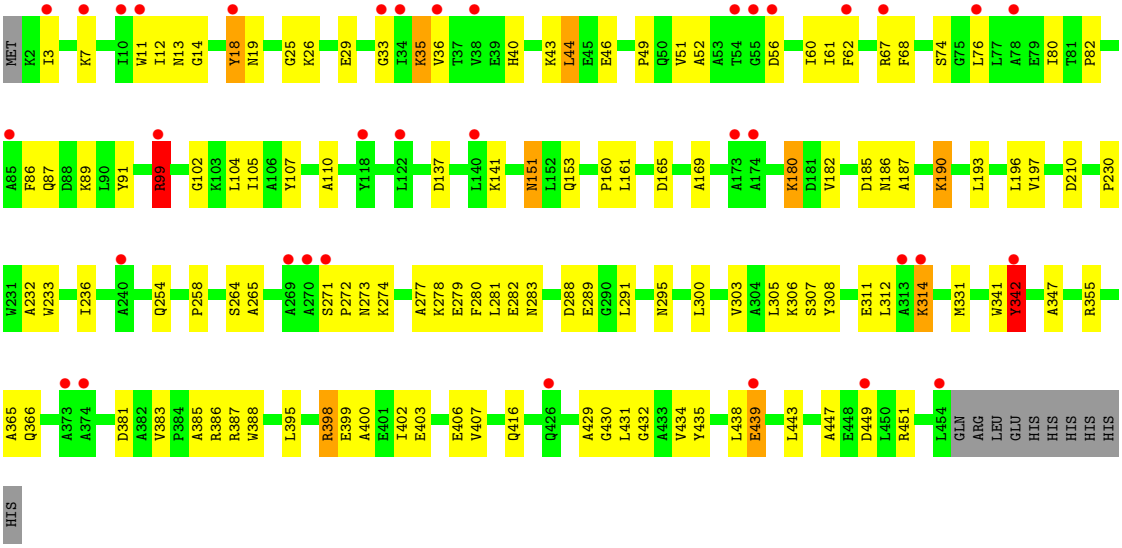
• Molecule 1: Maltose-binding periplasmic protein,Tumor necrosis factor receptor superfamily, member 25

Chain C:



• Molecule 1: Maltose-binding periplasmic protein,Tumor necrosis factor receptor superfamily, member 25

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.40Å 144.87Å 177.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 2.55 47.53 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.53-2.55) 99.5 (47.53-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.234 , 0.274 0.234 , 0.274	Depositor DCC
R_{free} test set	3771 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	67.0	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14119	wwPDB-VP
Average B, all atoms (Å^2)	86.0	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 21.53 % 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 6.8724e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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	0.39	0/3562	0.72	10/4835 (0.2%)
1	B	0.38	0/3579	0.67	6/4857 (0.1%)
1	C	0.52	2/3570 (0.1%)	0.92	22/4845 (0.5%)
1	D	0.47	1/3596 (0.0%)	0.77	15/4879 (0.3%)
All	All	0.44	3/14307 (0.0%)	0.77	53/19416 (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	B	0	1
1	C	0	1
1	D	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	355	ARG	CB-CG	-7.60	1.32	1.52
1	C	51	VAL	CB-CG1	5.64	1.64	1.52
1	D	439	GLU	CD-OE2	5.50	1.31	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	355	ARG	NE-CZ-NH2	-26.89	106.86	120.30
1	D	99	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	C	355	ARG	NE-CZ-NH1	10.43	125.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	312	LEU	CB-CG-CD1	9.46	127.09	111.00
1	D	35	LYS	CA-CB-CG	-9.34	92.86	113.40
1	D	439	GLU	CA-CB-CG	9.29	133.83	113.40
1	D	342	TYR	CB-CG-CD2	-9.05	115.57	121.00
1	C	139	GLU	CA-CB-CG	-8.96	93.69	113.40
1	C	67	ARG	CG-CD-NE	-8.88	93.14	111.80
1	B	171	LYS	CD-CE-NZ	8.85	132.06	111.70
1	D	67	ARG	CA-CB-CG	-8.80	94.03	113.40
1	A	329	GLU	CB-CA-C	-8.68	93.04	110.40
1	C	10	ILE	CG1-CB-CG2	-8.33	93.08	111.40
1	A	444	GLU	CA-CB-CG	-7.94	95.93	113.40
1	C	38	VAL	CG1-CB-CG2	-7.86	98.32	110.90
1	D	35	LYS	CD-CE-NZ	-7.65	94.11	111.70
1	A	67	ARG	CG-CD-NE	7.60	127.77	111.80
1	A	26	LYS	CB-CG-CD	-7.47	92.17	111.60
1	B	171	LYS	CB-CG-CD	-7.47	92.19	111.60
1	D	99	ARG	CD-NE-CZ	7.17	133.65	123.60
1	A	329	GLU	N-CA-CB	7.09	123.37	110.60
1	B	10	ILE	CG1-CB-CG2	-6.94	96.14	111.40
1	A	67	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	C	355	ARG	NH1-CZ-NH2	6.59	126.64	119.40
1	C	56	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	D	439	GLU	CB-CA-C	6.39	123.18	110.40
1	C	386	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	C	306	LYS	N-CA-CB	-6.28	99.29	110.60
1	C	329	GLU	CA-CB-CG	-6.16	99.84	113.40
1	C	23	GLU	CA-CB-CG	6.05	126.70	113.40
1	B	171	LYS	CA-CB-CG	-5.98	100.25	113.40
1	D	190	LYS	N-CA-CB	-5.97	99.86	110.60
1	A	426	GLN	N-CA-CB	-5.93	99.92	110.60
1	A	329	GLU	CA-CB-CG	5.88	126.34	113.40
1	D	355	ARG	CA-CB-CG	-5.86	100.51	113.40
1	C	424	ARG	CB-CG-CD	-5.86	96.38	111.60
1	A	152	LEU	CA-CB-CG	5.81	128.67	115.30
1	C	141	LYS	CB-CG-CD	5.78	126.62	111.60
1	D	44	LEU	CA-CB-CG	5.76	128.54	115.30
1	C	51	VAL	CA-CB-CG2	-5.61	102.48	110.90
1	B	7	LYS	CA-CB-CG	5.58	125.67	113.40
1	C	141	LYS	CD-CE-NZ	-5.54	98.96	111.70
1	C	355	ARG	N-CA-CB	-5.50	100.70	110.60
1	C	56	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	355	ARG	CB-CG-CD	5.43	125.72	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	306	LYS	CA-CB-CG	5.43	125.34	113.40
1	C	30	LYS	CD-CE-NZ	5.39	124.09	111.70
1	C	312	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	D	355	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	314	LYS	CB-CG-CD	5.12	124.91	111.60
1	B	7	LYS	CB-CA-C	5.11	120.63	110.40
1	D	314	LYS	CG-CD-CE	-5.11	96.56	111.90
1	D	99	ARG	CB-CA-C	-5.03	100.35	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	28	PHE	Mainchain
1	C	139	GLU	Sidechain
1	D	342	TYR	Sidechain
1	D	99	ARG	Sidechain

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	3482	0	3445	87	0
1	B	3499	0	3463	107	0
1	C	3490	0	3457	137	0
1	D	3516	0	3487	104	0
2	A	30	0	0	2	0
2	B	40	0	0	1	0
2	C	25	0	0	1	0
2	D	35	0	0	1	0
3	B	2	0	0	0	0
All	All	14119	0	13852	417	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 15.

All (417) 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:401:GLU:OE2	1:C:426:GLN:NE2	1.88	1.06
1:B:453:ARG:HD2	1:D:386:ARG:HH12	1.21	1.04
1:D:43:LYS:NZ	1:D:439:GLU:OE1	1.91	1.04
1:C:401:GLU:CD	1:C:426:GLN:HE22	1.64	1.00
1:D:44:LEU:HD21	1:D:61:ILE:HD11	1.44	1.00
1:B:32:THR:HG23	1:B:34:ILE:H	1.21	0.99
1:C:9:VAL:HG23	1:C:58:PRO:HA	1.46	0.97
1:D:3:ILE:HD11	1:D:271:SER:HA	1.46	0.97
1:D:291:LEU:CD1	1:D:308:TYR:CD2	2.53	0.92
1:A:386:ARG:HH22	1:C:453:ARG:HH11	1.17	0.88
1:C:80:ILE:HD13	1:C:82:PRO:HD3	1.55	0.87
1:D:180:LYS:O	1:D:180:LYS:HD3	1.76	0.86
1:C:424:ARG:HH12	1:C:429:ALA:HA	1.43	0.84
1:C:51:VAL:HG12	1:C:56:ASP:HB3	1.59	0.83
1:A:378:ASP:HB3	1:C:386:ARG:HH12	1.43	0.83
1:B:10:ILE:O	1:B:10:ILE:HD12	1.79	0.82
1:D:291:LEU:HD13	1:D:308:TYR:CD2	2.14	0.82
1:D:3:ILE:HD11	1:D:272:PRO:HD3	1.62	0.82
1:B:80:ILE:HD11	1:B:95:TRP:HZ3	1.46	0.81
1:C:60:ILE:HD11	1:C:277:ALA:HB1	1.62	0.81
1:A:216:ALA:O	1:A:220:LYS:HG3	1.81	0.81
1:D:3:ILE:CD1	1:D:271:SER:HA	2.10	0.80
1:C:63:TRP:HE1	1:C:67:ARG:HH21	1.25	0.80
1:D:80:ILE:HG23	1:D:82:PRO:HD3	1.63	0.80
1:B:43:LYS:HE3	1:B:451:ARG:HD3	1.63	0.79
1:C:63:TRP:HE1	1:C:67:ARG:NH2	1.81	0.78
1:C:51:VAL:HG12	1:C:56:ASP:CB	2.13	0.78
1:A:243:TYR:OH	1:A:317:ARG:NH1	2.17	0.77
1:C:219:ASN:OD1	1:C:236:ILE:HD12	1.85	0.77
1:B:32:THR:HG23	1:B:34:ILE:N	1.99	0.76
1:D:82:PRO:HA	1:D:278:LYS:HZ1	1.49	0.76
1:C:22:ALA:HB2	1:C:38:VAL:HG11	1.68	0.76
1:C:424:ARG:HE	1:C:424:ARG:HA	1.51	0.75
1:B:80:ILE:HG13	1:B:82:PRO:HD3	1.67	0.75
1:C:52:ALA:HB3	1:C:76:LEU:HD23	1.69	0.74
1:B:453:ARG:HD2	1:D:386:ARG:NH1	2.00	0.74
1:C:424:ARG:NH2	1:C:427:GLN:O	2.21	0.74
1:D:182:VAL:O	1:D:366:GLN:NE2	2.22	0.72
1:C:32:THR:HG23	1:C:34:ILE:H	1.56	0.71
1:D:186:ASN:O	1:D:190:LYS:HB2	1.90	0.71
1:A:322:MET:HG3	1:A:326:GLN:HE21	1.55	0.71
1:A:424:ARG:NH2	2:A:502:SO4:O1	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ARG:NH1	1:D:449:ASP:OD2	2.24	0.70
1:B:29:GLU:HA	1:B:32:THR:HG22	1.72	0.70
1:C:295:ASN:OD1	1:C:299:PRO:HA	1.92	0.70
1:A:306:LYS:O	1:A:310:GLU:HG3	1.91	0.70
1:D:291:LEU:HD11	1:D:308:TYR:CD2	2.26	0.70
1:A:67:ARG:HG3	1:A:71:TYR:CZ	2.27	0.69
1:B:23:GLU:HA	1:B:26:LYS:HE2	1.73	0.69
1:A:166:GLY:O	1:A:186:ASN:ND2	2.24	0.69
1:C:392:VAL:HG22	1:C:397:LEU:HD23	1.75	0.69
1:C:8:LEU:HB2	1:C:36:VAL:HG12	1.74	0.69
1:C:80:ILE:CD1	1:C:82:PRO:HD3	2.21	0.69
1:D:187:ALA:N	2:D:507:SO4:O1	2.26	0.68
1:C:328:GLY:C	1:C:329:GLU:HG2	2.13	0.68
1:C:51:VAL:CG1	1:C:56:ASP:HB3	2.22	0.68
1:B:386:ARG:HG3	1:D:381:ASP:O	1.93	0.68
1:D:311:GLU:OE2	1:D:314:LYS:NZ	2.26	0.68
1:D:44:LEU:CD2	1:D:61:ILE:HD11	2.21	0.68
1:A:444:GLU:OE1	1:A:444:GLU:N	2.21	0.67
1:B:435:TYR:HB3	1:B:451:ARG:HH21	1.58	0.67
1:A:179:ILE:HD11	1:A:336:GLN:NE2	2.09	0.67
1:A:255:PRO:HB3	1:A:327:LYS:HD3	1.77	0.67
1:C:424:ARG:NH1	1:C:429:ALA:CA	2.57	0.67
1:C:178:ASP:OD1	1:C:180:LYS:HD3	1.95	0.67
1:B:60:ILE:HG12	1:B:267:ILE:HG22	1.77	0.66
1:D:51:VAL:HG13	1:D:56:ASP:HB3	1.77	0.66
1:A:61:ILE:HD12	1:A:61:ILE:O	1.95	0.66
1:B:22:ALA:O	1:B:26:LYS:HG3	1.95	0.66
1:C:401:GLU:CD	1:C:426:GLN:NE2	2.44	0.66
1:D:80:ILE:HD11	1:D:107:TYR:CE2	2.31	0.65
1:C:424:ARG:HH12	1:C:429:ALA:CA	2.10	0.65
1:D:44:LEU:HD21	1:D:61:ILE:CD1	2.23	0.65
1:D:80:ILE:HD11	1:D:107:TYR:CD2	2.32	0.65
1:A:386:ARG:HH22	1:C:453:ARG:NH1	1.94	0.65
1:B:80:ILE:HD11	1:B:95:TRP:CZ3	2.31	0.65
1:C:308:TYR:CZ	1:C:312:LEU:HD11	2.31	0.65
1:D:7:LYS:O	1:D:273:ASN:ND2	2.30	0.64
1:B:28:PHE:O	1:B:32:THR:HG22	1.97	0.64
1:A:236:ILE:HD11	1:A:243:TYR:CD2	2.33	0.64
1:C:217:ALA:O	1:C:222:GLU:HB2	1.99	0.63
1:B:397:LEU:HD13	1:B:423:TRP:HB2	1.81	0.63
1:A:236:ILE:HA	1:A:239:SER:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ARG:NH1	1:C:429:ALA:HA	2.14	0.63
1:B:10:ILE:CD1	1:B:38:VAL:HG23	2.29	0.62
1:A:11:TRP:HB2	1:A:61:ILE:HG22	1.81	0.62
1:A:67:ARG:HG3	1:A:71:TYR:CE1	2.34	0.62
1:C:50:GLN:NE2	1:C:431:LEU:O	2.32	0.62
1:B:413:ARG:NH2	1:C:414:ASP:OD2	2.28	0.62
1:C:13:ASN:OD1	1:C:14:GLY:N	2.32	0.62
1:A:187:ALA:N	2:A:506:SO4:O2	2.31	0.62
1:D:279:GLU:HG3	1:D:283:ASN:HD22	1.64	0.61
1:C:10:ILE:HG12	1:C:60:ILE:HB	1.82	0.61
1:A:151:ASN:ND2	1:A:153:GLN:H	1.98	0.61
1:B:398:ARG:NH1	1:B:401:GLU:OE1	2.34	0.61
1:B:248:LEU:H	1:B:324:ASN:HD21	1.48	0.61
1:C:308:TYR:CZ	1:C:312:LEU:CD1	2.83	0.61
1:D:13:ASN:OD1	1:D:14:GLY:N	2.34	0.61
1:B:171:LYS:HG3	1:B:172:TYR:N	2.15	0.61
1:B:418:GLU:HA	1:B:418:GLU:OE1	2.00	0.61
1:D:137:ASP:OD2	1:D:141:LYS:HE2	2.00	0.60
1:C:26:LYS:O	1:C:29:GLU:HB3	2.00	0.60
1:A:7:LYS:NZ	1:A:35:LYS:H	2.00	0.60
1:B:401:GLU:OE2	1:B:426:GLN:NE2	2.34	0.60
1:B:32:THR:CG2	1:B:34:ILE:H	2.05	0.60
1:D:185:ASP:OD1	1:D:190:LYS:NZ	2.35	0.60
1:C:401:GLU:OE1	1:C:426:GLN:OE1	2.19	0.60
1:A:67:ARG:CG	1:A:71:TYR:CZ	2.86	0.59
1:C:80:ILE:HD12	1:C:80:ILE:O	2.01	0.59
1:C:52:ALA:CB	1:C:76:LEU:HD23	2.31	0.59
1:B:74:SER:HB2	1:B:76:LEU:HD13	1.82	0.59
1:A:56:ASP:OD2	1:A:57:GLY:N	2.30	0.59
1:B:44:LEU:HD13	1:B:61:ILE:HD11	1.84	0.59
1:B:236:ILE:CD1	1:B:243:TYR:CG	2.86	0.58
1:C:309:GLU:O	1:C:313:ALA:N	2.30	0.58
1:C:424:ARG:NH1	1:C:429:ALA:HB2	2.17	0.58
1:D:86:PHE:CZ	1:D:282:GLU:HG2	2.38	0.58
1:A:442:GLY:C	1:A:444:GLU:OE1	2.42	0.58
1:C:63:TRP:HA	1:C:63:TRP:CE3	2.38	0.58
1:D:43:LYS:HE3	1:D:451:ARG:HH12	1.69	0.58
1:B:9:VAL:HG13	1:B:58:PRO:HA	1.86	0.58
1:B:383:VAL:HG12	1:B:438:LEU:HD21	1.85	0.58
1:C:34:ILE:HG21	1:C:276:LEU:HD13	1.86	0.58
1:D:43:LYS:HE3	1:D:451:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:ILE:HD11	1:D:272:PRO:CD	2.33	0.57
1:D:289:GLU:H	1:D:289:GLU:CD	2.05	0.57
1:C:295:ASN:ND2	1:C:296:LYS:HZ2	2.02	0.57
1:C:80:ILE:HD12	1:C:80:ILE:C	2.24	0.56
1:C:428:PRO:O	1:C:431:LEU:HD12	2.05	0.56
1:D:291:LEU:HD11	1:D:308:TYR:CG	2.39	0.56
1:C:51:VAL:HG12	1:C:57:GLY:N	2.21	0.56
1:B:93:PHE:HD2	1:B:330:ILE:HD11	1.71	0.56
1:A:332:PRO:HB2	1:A:337:MET:HE3	1.87	0.56
1:B:236:ILE:HD13	1:B:243:TYR:CG	2.41	0.56
1:D:185:ASP:O	1:D:190:LYS:NZ	2.37	0.56
1:B:236:ILE:HA	1:B:239:SER:HB3	1.87	0.56
1:C:453:ARG:HG3	1:C:453:ARG:O	2.06	0.56
1:C:295:ASN:ND2	1:C:296:LYS:NZ	2.54	0.55
1:C:392:VAL:CG2	1:C:397:LEU:HD23	2.35	0.55
1:A:150:PHE:O	1:A:152:LEU:HD22	2.07	0.55
1:C:424:ARG:HH11	1:C:429:ALA:HB2	1.71	0.55
1:D:447:ALA:O	1:D:451:ARG:N	2.38	0.55
1:C:22:ALA:HB2	1:C:38:VAL:CG1	2.36	0.55
1:C:230:PRO:HA	1:C:233:TRP:CE2	2.42	0.55
1:D:151:ASN:ND2	1:D:153:GLN:H	2.05	0.55
1:A:11:TRP:CD2	1:A:58:PRO:HG3	2.42	0.54
1:A:336:GLN:OE1	1:A:336:GLN:N	2.27	0.54
1:C:141:LYS:HG2	1:C:145:LYS:O	2.07	0.54
1:D:435:TYR:O	1:D:439:GLU:HB3	2.07	0.54
1:B:150:PHE:O	1:B:152:LEU:HD12	2.07	0.54
1:C:383:VAL:HG12	1:C:438:LEU:HD21	1.90	0.54
1:C:273:ASN:HB3	1:C:276:LEU:HD12	1.90	0.54
1:A:336:GLN:H	1:A:336:GLN:CD	2.03	0.54
1:C:404:ALA:O	1:C:407:VAL:HG12	2.08	0.54
1:C:424:ARG:HA	1:C:424:ARG:NE	2.22	0.54
1:B:10:ILE:CD1	1:B:38:VAL:HA	2.37	0.54
1:D:82:PRO:HA	1:D:278:LYS:NZ	2.22	0.54
1:B:131:GLU:OE1	1:B:131:GLU:N	2.36	0.53
1:C:185:ASP:HB2	1:C:366:GLN:HB2	1.90	0.53
1:C:275:GLU:O	1:C:279:GLU:HG3	2.08	0.53
1:B:80:ILE:CD1	1:B:95:TRP:HZ3	2.18	0.53
1:A:287:THR:HG23	1:A:290:GLY:H	1.74	0.53
1:A:45:GLU:HG2	1:A:46:GLU:HG2	1.91	0.52
1:B:29:GLU:HA	1:B:32:THR:CG2	2.39	0.52
1:B:342:TYR:O	1:B:346:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ARG:HD2	1:D:399:GLU:H	1.75	0.52
1:B:10:ILE:HD11	1:B:38:VAL:HG23	1.91	0.52
1:B:407:VAL:HG21	1:C:356:GLN:NE2	2.25	0.52
1:C:435:TYR:O	1:C:439:GLU:HG3	2.10	0.52
1:A:408:GLU:O	1:D:342:TYR:OH	2.22	0.52
1:B:10:ILE:HD12	1:B:10:ILE:C	2.30	0.52
1:B:364:ALA:HB1	1:C:407:VAL:HG11	1.92	0.52
1:A:25:GLY:HA3	1:A:36:VAL:CG2	2.40	0.52
1:B:389:LYS:HA	1:B:392:VAL:HG22	1.92	0.52
1:B:398:ARG:NH1	1:B:401:GLU:CD	2.63	0.51
1:C:169:ALA:O	1:C:182:VAL:HG23	2.09	0.51
1:D:62:PHE:CE1	1:D:265:ALA:HB2	2.45	0.51
1:D:230:PRO:HA	1:D:233:TRP:CE2	2.45	0.51
1:B:78:ALA:HB3	1:B:267:ILE:HD11	1.91	0.51
1:C:40:HIS:O	1:C:40:HIS:ND1	2.43	0.51
1:D:347:ALA:HB2	1:D:365:ALA:HB2	1.92	0.51
1:D:402:ILE:O	1:D:406:GLU:HG3	2.09	0.51
1:B:25:GLY:CA	1:B:36:VAL:HG11	2.41	0.51
1:B:90:LEU:HD23	1:B:95:TRP:CZ2	2.46	0.51
1:B:46:GLU:CD	1:B:67:ARG:HH22	2.14	0.51
1:C:66:ASP:OD2	1:C:66:ASP:N	2.42	0.51
1:C:292:GLU:HG2	1:C:296:LYS:HZ3	1.75	0.51
1:D:169:ALA:O	1:D:182:VAL:HG23	2.10	0.51
1:B:25:GLY:HA3	1:B:36:VAL:HG11	1.93	0.51
1:A:275:GLU:O	1:A:279:GLU:HG3	2.11	0.50
1:C:7:LYS:HE3	1:C:9:VAL:HG12	1.93	0.50
1:B:22:ALA:HB2	1:B:38:VAL:HG11	1.93	0.50
1:A:142:ALA:C	1:A:143:LYS:HD3	2.32	0.50
1:C:295:ASN:HD22	1:C:296:LYS:NZ	2.09	0.50
1:D:18:TYR:CE1	1:D:19:ASN:ND2	2.79	0.50
1:B:50:GLN:NE2	1:B:431:LEU:O	2.35	0.50
1:D:80:ILE:HD11	1:D:107:TYR:CZ	2.47	0.50
1:A:25:GLY:HA3	1:A:36:VAL:HG21	1.94	0.50
1:B:211:TYR:HE1	1:B:228:ASN:HD21	1.60	0.50
1:B:236:ILE:CD1	1:B:243:TYR:CD2	2.95	0.50
1:D:60:ILE:HG21	1:D:281:LEU:HD11	1.94	0.50
1:B:401:GLU:CD	1:B:426:GLN:HE22	2.15	0.49
1:C:234:SER:O	1:C:238:THR:HG23	2.12	0.49
1:C:389:LYS:NZ	1:C:406:GLU:OE2	2.36	0.49
1:D:308:TYR:CE2	1:D:312:LEU:HD11	2.47	0.49
1:B:295:ASN:OD1	1:B:299:PRO:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ALA:HA	1:C:303:VAL:HA	1.94	0.49
1:D:278:LYS:NZ	1:D:282:GLU:OE2	2.45	0.49
1:D:383:VAL:HG22	1:D:438:LEU:HD21	1.94	0.49
1:B:421:LYS:NZ	2:B:502:SO4:O3	2.38	0.49
1:C:331:MET:SD	1:C:341:TRP:HZ2	2.36	0.49
1:C:424:ARG:NH1	2:C:504:SO4:O1	2.45	0.49
1:B:164:ALA:HB2	1:B:256:SER:HA	1.95	0.49
1:C:424:ARG:NH1	1:C:429:ALA:CB	2.75	0.49
1:D:165:ASP:HA	1:D:254:GLN:OE1	2.13	0.49
1:C:86:PHE:CZ	1:C:282:GLU:HG2	2.47	0.49
1:A:402:ILE:O	1:A:406:GLU:HG3	2.13	0.49
1:B:80:ILE:HG13	1:B:82:PRO:CD	2.39	0.49
1:B:350:ASN:HB3	1:B:355:ARG:HB3	1.94	0.49
1:D:46:GLU:OE1	1:D:432:GLY:HA2	2.13	0.49
1:D:151:ASN:ND2	1:D:210:ASP:HA	2.28	0.49
1:A:347:ALA:HB2	1:A:365:ALA:HB2	1.95	0.48
1:C:8:LEU:O	1:C:36:VAL:HA	2.12	0.48
1:A:314:LYS:HG2	1:A:315:ASP:H	1.78	0.48
1:C:11:TRP:HB3	1:C:44:LEU:HD13	1.93	0.48
1:B:45:GLU:HG2	1:B:46:GLU:HG2	1.95	0.48
1:C:44:LEU:HD11	1:C:61:ILE:CD1	2.44	0.48
1:D:271:SER:O	1:D:274:LYS:HG3	2.14	0.48
1:D:46:GLU:OE1	1:D:432:GLY:CA	2.61	0.48
1:A:56:ASP:CG	1:A:57:GLY:H	2.16	0.48
1:A:19:ASN:O	1:A:23:GLU:HG2	2.14	0.48
1:A:30:LYS:HG2	1:A:31:ASP:OD1	2.13	0.48
1:A:443:LEU:N	1:A:444:GLU:OE1	2.47	0.48
1:B:44:LEU:CD1	1:B:61:ILE:HD11	2.44	0.48
1:D:295:ASN:HD22	1:D:300:LEU:H	1.62	0.48
1:D:435:TYR:HB3	1:D:451:ARG:HH21	1.79	0.48
1:B:350:ASN:CB	1:B:355:ARG:HB3	2.44	0.48
1:A:297:ASP:O	1:A:298:LYS:HG2	2.13	0.47
1:B:90:LEU:HD23	1:B:95:TRP:HZ2	1.78	0.47
1:B:408:GLU:HG3	1:C:342:TYR:HE2	1.78	0.47
1:C:428:PRO:O	1:C:431:LEU:CD1	2.62	0.47
1:D:80:ILE:HG22	1:D:104:LEU:HB2	1.97	0.47
1:A:96:ASP:HA	1:A:99:ARG:HH12	1.78	0.47
1:D:35:LYS:HG3	1:D:36:VAL:N	2.28	0.47
1:B:408:GLU:HG3	1:C:342:TYR:CE2	2.50	0.47
1:C:28:PHE:HA	1:C:284:TYR:CE2	2.50	0.47
1:C:28:PHE:O	1:C:32:THR:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LYS:HE2	1:D:305:LEU:HD11	1.96	0.47
1:A:45:GLU:OE2	1:A:45:GLU:N	2.41	0.47
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.50	0.47
1:C:211:TYR:HE1	1:C:228:ASN:HD21	1.62	0.47
1:A:381:ASP:O	1:C:386:ARG:HB2	2.15	0.47
1:C:117:ILE:HD13	1:C:245:VAL:HG22	1.96	0.47
1:C:137:ASP:OD2	1:C:204:HIS:ND1	2.35	0.47
1:A:260:VAL:HG23	1:A:329:GLU:O	2.15	0.47
1:B:413:ARG:HH22	1:C:414:ASP:CG	2.18	0.47
1:D:68:PHE:HB3	1:D:105:ILE:HD13	1.97	0.47
1:C:9:VAL:CG2	1:C:58:PRO:HA	2.30	0.46
1:D:279:GLU:HG3	1:D:283:ASN:ND2	2.30	0.46
1:A:96:ASP:HA	1:A:99:ARG:NH1	2.30	0.46
1:B:398:ARG:O	1:B:401:GLU:HB2	2.15	0.46
1:C:89:LYS:O	1:C:306:LYS:HB3	2.15	0.46
1:D:232:ALA:O	1:D:236:ILE:HG12	2.14	0.46
1:A:7:LYS:HZ2	1:A:35:LYS:H	1.63	0.46
1:B:141:LYS:NZ	1:B:203:LYS:O	2.49	0.46
1:A:93:PHE:O	1:A:330:ILE:HD11	2.15	0.46
1:B:10:ILE:HD11	1:B:38:VAL:HA	1.96	0.46
1:B:289:GLU:H	1:B:289:GLU:CD	2.19	0.46
1:D:193:LEU:O	1:D:197:VAL:HG13	2.15	0.46
1:B:68:PHE:HB3	1:B:105:ILE:HD13	1.97	0.46
1:B:80:ILE:CG1	1:B:82:PRO:HD3	2.41	0.46
1:D:29:GLU:O	1:D:33:GLY:N	2.45	0.46
1:C:60:ILE:HD11	1:C:277:ALA:CB	2.37	0.46
1:C:308:TYR:O	1:C:311:GLU:HB3	2.15	0.46
1:C:355:ARG:HH21	1:C:355:ARG:HD2	1.26	0.46
1:D:288:ASP:OD1	1:D:307:SER:OG	2.23	0.46
1:A:296:LYS:O	1:A:296:LYS:HG3	2.16	0.46
1:C:402:ILE:HG23	1:C:419:MET:HE1	1.98	0.46
1:A:69:GLY:HA3	1:A:333:ASN:O	2.16	0.46
1:B:402:ILE:O	1:B:406:GLU:HG3	2.16	0.46
1:B:398:ARG:HH12	1:B:401:GLU:CD	2.18	0.46
1:A:219:ASN:OD1	1:A:236:ILE:HG22	2.17	0.45
1:B:350:ASN:CG	1:B:355:ARG:HG2	2.36	0.45
1:B:233:TRP:O	1:B:236:ILE:HG13	2.15	0.45
1:A:236:ILE:HD11	1:A:243:TYR:CE2	2.50	0.45
1:A:259:PHE:HA	1:A:329:GLU:HG2	1.98	0.45
1:B:332:PRO:HB2	1:B:337:MET:HE3	1.98	0.45
1:B:388:TRP:CE2	1:B:416:GLN:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ILE:CD1	1:C:245:VAL:HG22	2.45	0.45
1:D:80:ILE:HD11	1:D:107:TYR:CG	2.51	0.45
1:D:311:GLU:O	1:D:314:LYS:HG2	2.16	0.45
1:C:46:GLU:OE2	1:C:451:ARG:NH1	2.50	0.45
1:C:119:ASN:CG	1:C:122:LEU:HD12	2.36	0.45
1:D:12:ILE:O	1:D:40:HIS:HA	2.17	0.45
1:B:171:LYS:HD2	1:B:171:LYS:HA	1.63	0.45
1:A:259:PHE:CD1	1:A:329:GLU:CG	3.00	0.45
1:D:395:LEU:HD21	1:D:434:VAL:HA	1.98	0.45
1:D:49:PRO:HB2	1:D:431:LEU:HB3	1.98	0.45
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.52	0.45
1:B:8:LEU:HA	1:B:59:ASP:OD2	2.17	0.45
1:D:161:LEU:HD23	1:D:196:LEU:HB2	1.99	0.45
1:A:47:LYS:O	1:A:51:VAL:HG22	2.17	0.44
1:A:89:LYS:HE2	1:A:305:LEU:HD11	1.99	0.44
1:C:50:GLN:O	1:C:54:THR:HG23	2.17	0.44
1:D:91:TYR:CZ	1:D:306:LYS:HA	2.52	0.44
1:D:331:MET:SD	1:D:341:TRP:HZ2	2.40	0.44
1:D:398:ARG:NH2	1:D:400:ALA:HB2	2.32	0.44
1:B:418:GLU:OE1	1:B:421:LYS:HE2	2.17	0.44
1:C:86:PHE:CE2	1:C:282:GLU:HG2	2.52	0.44
1:C:305:LEU:HD23	1:C:307:SER:H	1.82	0.44
1:B:10:ILE:HD12	1:B:38:VAL:HA	1.99	0.44
1:B:15:ASP:OD1	1:B:15:ASP:N	2.47	0.44
1:B:19:ASN:HB2	1:B:297:ASP:OD2	2.17	0.44
1:A:155:PRO:HG2	1:A:341:TRP:CE3	2.52	0.44
1:A:408:GLU:HG3	1:A:409:ILE:HG12	1.98	0.44
1:B:32:THR:HG23	1:B:33:GLY:N	2.32	0.44
1:B:69:GLY:HA3	1:B:333:ASN:O	2.17	0.44
1:A:58:PRO:HG2	1:A:61:ILE:HG23	1.98	0.44
1:C:424:ARG:O	1:C:427:GLN:O	2.36	0.44
1:C:429:ALA:HA	1:C:430:GLY:HA2	1.69	0.44
1:A:346:THR:HG21	1:D:407:VAL:HG22	2.00	0.44
1:B:7:LYS:O	1:B:273:ASN:ND2	2.51	0.44
1:D:18:TYR:CD2	1:D:40:HIS:CD2	3.06	0.44
1:D:110:ALA:HA	1:D:303:VAL:HA	2.00	0.44
1:A:378:ASP:CB	1:C:386:ARG:HH12	2.22	0.44
1:C:359:ASP:OD1	1:C:360:ALA:N	2.50	0.44
1:D:74:SER:HB2	1:D:76:LEU:HD13	2.00	0.44
1:D:82:PRO:HG2	1:D:87:GLN:HE21	1.83	0.44
1:A:91:TYR:CZ	1:A:306:LYS:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLY:HA2	1:A:298:LYS:HG3	1.99	0.43
1:A:141:LYS:NZ	1:A:203:LYS:O	2.51	0.43
1:C:7:LYS:HE3	1:C:9:VAL:CG1	2.48	0.43
1:D:26:LYS:HB2	1:D:26:LYS:HE2	1.77	0.43
1:D:99:ARG:NH1	1:D:102:GLY:HA2	2.33	0.43
1:D:291:LEU:HD13	1:D:308:TYR:CE2	2.51	0.43
1:D:387:ARG:NH1	1:D:443:LEU:HD21	2.33	0.43
1:A:13:ASN:OD1	1:A:14:GLY:N	2.51	0.43
1:B:22:ALA:HB2	1:B:38:VAL:CG1	2.49	0.43
1:C:388:TRP:CE2	1:C:416:GLN:HG2	2.53	0.43
1:B:44:LEU:HA	1:B:47:LYS:HG2	2.01	0.43
1:A:28:PHE:CE2	1:A:34:ILE:HB	2.53	0.43
1:C:401:GLU:OE1	1:C:426:GLN:NE2	2.51	0.43
1:D:279:GLU:CG	1:D:283:ASN:HD22	2.31	0.43
1:B:61:ILE:HD12	1:B:62:PHE:N	2.34	0.43
1:D:160:PRO:HG3	1:D:258:PRO:HA	2.00	0.43
1:A:7:LYS:O	1:A:273:ASN:ND2	2.52	0.43
1:A:8:LEU:HB2	1:A:36:VAL:HG12	2.00	0.43
1:A:52:ALA:HA	1:A:56:ASP:O	2.18	0.43
1:C:80:ILE:HD11	1:C:104:LEU:HB2	2.01	0.43
1:D:25:GLY:HA3	1:D:36:VAL:HG21	2.01	0.43
1:B:359:ASP:OD1	1:B:360:ALA:N	2.52	0.42
1:C:44:LEU:HD11	1:C:61:ILE:HD11	2.01	0.42
1:C:257:LYS:HG2	1:C:327:LYS:O	2.19	0.42
1:C:12:ILE:O	1:C:40:HIS:HA	2.19	0.42
1:D:388:TRP:HB3	1:D:416:GLN:OE1	2.19	0.42
1:C:136:LEU:O	1:C:140:LEU:HG	2.20	0.42
1:D:403:GLU:O	1:D:407:VAL:HG12	2.19	0.42
1:A:11:TRP:CG	1:A:58:PRO:HG3	2.54	0.42
1:A:387:ARG:HH21	1:A:390:GLU:CD	2.22	0.42
1:C:51:VAL:HG12	1:C:56:ASP:C	2.39	0.42
1:D:60:ILE:HD11	1:D:277:ALA:HB1	2.01	0.42
1:A:7:LYS:HE3	1:A:35:LYS:O	2.19	0.42
1:C:11:TRP:HB3	1:C:44:LEU:CD1	2.50	0.42
1:C:80:ILE:HD11	1:C:104:LEU:CB	2.49	0.42
1:C:392:VAL:HG11	1:C:419:MET:CE	2.49	0.42
1:D:169:ALA:O	1:D:182:VAL:HA	2.19	0.42
1:B:172:TYR:HB2	1:B:177:TYR:CE1	2.54	0.42
1:C:82:PRO:HA	1:C:282:GLU:OE2	2.20	0.42
1:A:28:PHE:HA	1:A:284:TYR:CE2	2.55	0.42
1:A:152:LEU:HD23	1:A:209:THR:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASP:O	1:C:141:LYS:HG3	2.19	0.42
1:C:25:GLY:HA2	1:C:280:PHE:CE1	2.55	0.42
1:C:8:LEU:HA	1:C:59:ASP:OD2	2.20	0.42
1:B:387:ARG:NH2	1:B:441:MET:HB3	2.35	0.41
1:D:429:ALA:HA	1:D:430:GLY:HA2	1.80	0.41
1:D:82:PRO:CA	1:D:278:LYS:HZ1	2.28	0.41
1:A:68:PHE:HB3	1:A:105:ILE:HD13	2.02	0.41
1:A:154:GLU:OE1	1:A:345:ARG:HD2	2.21	0.41
1:B:165:ASP:HA	1:B:254:GLN:OE1	2.21	0.41
1:C:292:GLU:HG2	1:C:296:LYS:NZ	2.35	0.41
1:C:389:LYS:HA	1:C:392:VAL:HG12	2.03	0.41
1:C:195:PHE:O	1:C:199:LEU:HD13	2.20	0.41
1:C:328:GLY:O	1:C:329:GLU:HG2	2.20	0.41
1:C:63:TRP:HA	1:C:63:TRP:HE3	1.85	0.41
1:D:62:PHE:HA	1:D:264:SER:O	2.20	0.41
1:D:385:ALA:HA	1:D:388:TRP:CE2	2.56	0.41
1:A:388:TRP:HB3	1:A:416:GLN:OE1	2.21	0.41
1:C:295:ASN:HB3	1:C:296:LYS:HZ3	1.84	0.41
1:A:137:ASP:OD2	1:A:141:LYS:HD2	2.21	0.41
1:C:80:ILE:HD13	1:C:82:PRO:CD	2.39	0.41
1:C:305:LEU:HD23	1:C:306:LYS:N	2.34	0.41
1:D:52:ALA:HA	1:D:56:ASP:O	2.20	0.41
1:A:346:THR:O	1:A:349:ILE:HG13	2.21	0.41
1:B:52:ALA:HA	1:B:56:ASP:O	2.20	0.41
1:B:61:ILE:HD12	1:B:62:PHE:H	1.85	0.41
1:B:350:ASN:OD1	1:B:355:ARG:HG2	2.21	0.41
1:C:137:ASP:HA	1:C:147:ALA:HB2	2.02	0.41
1:C:308:TYR:OH	1:C:312:LEU:HD11	2.20	0.41
1:B:25:GLY:O	1:B:28:PHE:HB3	2.20	0.41
1:B:73:GLN:HA	1:B:73:GLN:NE2	2.36	0.41
1:B:81:THR:O	1:B:81:THR:OG1	2.32	0.41
1:B:236:ILE:HD11	1:B:243:TYR:CG	2.56	0.41
1:D:3:ILE:HG22	1:D:56:ASP:HA	2.02	0.41
1:C:51:VAL:CG1	1:C:56:ASP:CB	2.89	0.40
1:C:296:LYS:HA	1:C:296:LYS:HD3	1.81	0.40
1:D:11:TRP:HB3	1:D:44:LEU:HD11	2.02	0.40
1:D:35:LYS:CG	1:D:36:VAL:N	2.83	0.40
1:D:25:GLY:HA2	1:D:280:PHE:CE1	2.56	0.40
1:A:141:LYS:HA	1:A:145:LYS:O	2.21	0.40
1:A:356:GLN:HG2	1:D:403:GLU:OE1	2.21	0.40
1:B:13:ASN:ND2	1:B:15:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HA	1:B:47:LYS:CG	2.51	0.40
1:A:7:LYS:HD2	1:A:7:LYS:HA	1.79	0.40
1:A:130:TRP:HB3	1:A:195:PHE:CE2	2.56	0.40
1:C:10:ILE:HD13	1:C:10:ILE:HG21	1.72	0.40
1:C:247:VAL:HA	1:C:324:ASN:HD21	1.87	0.40
1:B:245:VAL:HG12	1:B:320:ALA:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/464 (96%)	434 (97%)	13 (3%)	0	100	100
1	B	449/464 (97%)	434 (97%)	15 (3%)	0	100	100
1	C	448/464 (97%)	434 (97%)	14 (3%)	0	100	100
1	D	451/464 (97%)	436 (97%)	15 (3%)	0	100	100
All	All	1795/1856 (97%)	1738 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	349/364 (96%)	345 (99%)	4 (1%)	73	83
1	B	351/364 (96%)	349 (99%)	2 (1%)	86	92
1	C	350/364 (96%)	346 (99%)	4 (1%)	73	83
1	D	353/364 (97%)	348 (99%)	5 (1%)	67	79
All	All	1403/1456 (96%)	1388 (99%)	15 (1%)	73	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	180	LYS
1	A	426	GLN
1	A	451	ARG
1	B	314	LYS
1	B	355	ARG
1	C	45	GLU
1	C	180	LYS
1	C	292	GLU
1	C	296	LYS
1	D	18	TYR
1	D	99	ARG
1	D	151	ASN
1	D	180	LYS
1	D	398	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	326	GLN
1	B	153	GLN
1	B	242	ASN
1	B	324	ASN
1	C	295	ASN
1	C	426	GLN
1	D	19	ASN
1	D	87	GLN
1	D	125	ASN
1	D	151	ASN
1	D	206	ASN

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Mol	Chain	Res	Type
1	D	283	ASN
1	D	295	ASN
1	D	375	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

26 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	B	502	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	A	502	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	D	506	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	506	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	B	505	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	506	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	D	507	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	503	-	4,4,4	0.15	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	505	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	A	504	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	C	504	-	4,4,4	0.16	0	6,6,6	0.26	0
2	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	508	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	D	504	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	D	501	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	C	502	-	4,4,4	0.09	0	6,6,6	0.10	0
2	SO4	B	507	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	D	502	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	B	501	-	4,4,4	0.13	0	6,6,6	0.20	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.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	SO4	1	0
2	A	502	SO4	1	0
2	A	506	SO4	1	0
2	D	507	SO4	1	0
2	C	504	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	449/464 (96%)	0.64	31 (6%)	16	20	54, 80, 115, 170	0
1	B	451/464 (97%)	0.65	27 (5%)	21	25	55, 77, 113, 149	0
1	C	450/464 (96%)	0.93	57 (12%)	3	4	54, 89, 130, 162	0
1	D	453/464 (97%)	0.73	36 (7%)	12	16	54, 81, 128, 157	0
All	All	1803/1856 (97%)	0.74	151 (8%)	11	13	54, 81, 125, 170	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	454	LEU	7.1
1	C	37	THR	6.1
1	C	54	THR	5.7
1	C	431	LEU	5.7
1	C	21	LEU	5.6
1	C	18	TYR	5.4
1	A	173	ALA	4.9
1	B	243	TYR	4.8
1	A	180	LYS	4.8
1	A	123	LEU	4.6
1	C	34	ILE	4.4
1	C	291	LEU	4.4
1	C	312	LEU	4.4
1	C	174	ALA	4.3
1	C	269	ALA	4.2
1	C	5	GLU	4.1
1	D	99	ARG	4.1
1	B	174	ALA	4.1
1	D	3	ILE	4.0
1	C	117	ILE	4.0
1	C	237	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	270	ALA	4.0
1	B	33	GLY	3.9
1	D	342	TYR	3.8
1	C	240	ALA	3.8
1	D	54	THR	3.7
1	D	449	ASP	3.7
1	A	226	THR	3.6
1	C	53	ALA	3.6
1	C	19	ASN	3.6
1	A	6	GLY	3.5
1	D	34	ILE	3.5
1	C	124	PRO	3.5
1	C	270	ALA	3.4
1	A	124	PRO	3.3
1	B	453	ARG	3.3
1	C	342	TYR	3.2
1	B	136	LEU	3.1
1	C	7	LYS	3.1
1	B	55	GLY	3.1
1	C	300	LEU	3.1
1	C	243	TYR	3.1
1	B	240	ALA	3.1
1	C	61	ILE	3.0
1	D	426	GLN	3.0
1	A	175	GLY	3.0
1	A	122	LEU	3.0
1	A	3	ILE	3.0
1	D	173	ALA	3.0
1	D	62	PHE	3.0
1	C	35	LYS	3.0
1	D	313	ALA	2.9
1	C	60	ILE	2.9
1	C	272	PRO	2.9
1	D	10	ILE	2.9
1	B	291	LEU	2.9
1	C	308	TYR	2.9
1	C	62	PHE	2.8
1	C	242	ASN	2.8
1	C	41	PRO	2.8
1	A	241	VAL	2.8
1	A	176	LYS	2.8
1	A	426	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	180	LYS	2.7
1	A	171	LYS	2.7
1	C	241	VAL	2.7
1	D	36	VAL	2.7
1	D	174	ALA	2.7
1	A	329	GLU	2.7
1	D	18	TYR	2.7
1	D	122	LEU	2.7
1	D	439	GLU	2.6
1	C	105	ILE	2.6
1	D	240	ALA	2.6
1	D	33	GLY	2.6
1	B	118	TYR	2.6
1	B	342	TYR	2.6
1	C	277	ALA	2.6
1	C	47	LYS	2.6
1	D	314	LYS	2.6
1	C	280	PHE	2.6
1	A	118	TYR	2.6
1	B	220	LYS	2.5
1	B	117	ILE	2.5
1	D	78	ALA	2.5
1	D	85	ALA	2.5
1	C	28	PHE	2.5
1	A	243	TYR	2.5
1	A	435	TYR	2.5
1	A	37	THR	2.5
1	B	341	TRP	2.5
1	B	435	TYR	2.5
1	D	140	LEU	2.4
1	C	429	ALA	2.4
1	C	454	LEU	2.4
1	C	9	VAL	2.4
1	D	118	TYR	2.4
1	A	236	ILE	2.4
1	B	318	ILE	2.4
1	D	76	LEU	2.4
1	A	7	LYS	2.4
1	C	266	GLY	2.4
1	C	123	LEU	2.4
1	C	268	ASN	2.4
1	D	38	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	311	GLU	2.4
1	D	271	SER	2.3
1	B	97	ALA	2.3
1	B	54	THR	2.3
1	B	171	LYS	2.3
1	C	121	ASP	2.3
1	C	11	TRP	2.3
1	B	100	TYR	2.3
1	C	118	TYR	2.3
1	C	145	LYS	2.2
1	B	426	GLN	2.2
1	D	55	GLY	2.2
1	C	63	TRP	2.2
1	C	233	TRP	2.2
1	A	341	TRP	2.2
1	B	241	VAL	2.2
1	C	306	LYS	2.2
1	A	239	SER	2.2
1	C	434	VAL	2.2
1	C	56	ASP	2.2
1	A	320	ALA	2.1
1	C	139	GLU	2.1
1	A	26	LYS	2.1
1	B	18	TYR	2.1
1	B	53	ALA	2.1
1	B	83	ALA	2.1
1	D	269	ALA	2.1
1	D	373	ALA	2.1
1	C	305	LEU	2.1
1	A	225	MET	2.1
1	A	179	ILE	2.1
1	A	136	LEU	2.1
1	D	67	ARG	2.1
1	D	7	LYS	2.1
1	A	420	LEU	2.1
1	D	11	TRP	2.1
1	B	314	LYS	2.1
1	D	56	ASP	2.1
1	C	120	LYS	2.1
1	A	174	ALA	2.1
1	B	124	PRO	2.1
1	A	121	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	5	GLU	2.0
1	D	374	ALA	2.0
1	C	25	GLY	2.0
1	C	30	LYS	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 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(Å^2)	Q<0.9
2	SO4	A	506	5/5	0.76	0.29	160,161,162,162	0
2	SO4	D	504	5/5	0.76	0.21	142,142,143,144	0
2	SO4	D	507	5/5	0.81	0.24	124,125,126,127	0
2	SO4	B	508	5/5	0.82	0.22	145,145,145,146	0
2	SO4	B	504	5/5	0.86	0.17	143,143,144,144	0
2	SO4	D	505	5/5	0.89	0.23	127,128,128,128	0
2	SO4	A	504	5/5	0.89	0.21	133,134,134,135	0
2	SO4	A	503	5/5	0.91	0.13	123,124,125,125	0
2	SO4	B	501	5/5	0.91	0.19	85,86,87,87	0
2	SO4	C	504	5/5	0.91	0.13	132,133,134,134	0
2	SO4	B	505	5/5	0.92	0.18	114,115,115,115	0
2	SO4	B	506	5/5	0.92	0.18	130,130,132,133	0
2	SO4	B	507	5/5	0.92	0.17	134,135,135,135	0
2	SO4	D	506	5/5	0.92	0.23	115,116,117,118	0
2	SO4	B	502	5/5	0.92	0.13	107,108,109,110	0
2	SO4	A	505	5/5	0.93	0.22	145,146,146,147	0
2	SO4	C	505	5/5	0.93	0.14	136,137,138,138	0
2	SO4	C	503	5/5	0.93	0.15	120,120,121,123	0
2	SO4	B	503	5/5	0.94	0.12	118,118,118,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	503	5/5	0.94	0.14	128,128,128,130	0
2	SO4	A	502	5/5	0.94	0.24	83,85,87,87	0
2	SO4	C	501	5/5	0.96	0.18	63,65,67,70	0
2	SO4	D	502	5/5	0.97	0.16	86,87,87,89	0
2	SO4	D	501	5/5	0.97	0.17	66,67,69,69	0
2	SO4	A	501	5/5	0.98	0.16	69,70,70,71	0
2	SO4	C	502	5/5	0.98	0.19	60,62,65,68	0

6.5 Other polymers (i)

There are no such residues in this entry.