



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:24 AM GMT

PDB ID : 3IAD  
Title : Crystal structure of human phosphodiesterase 4D with bound allosteric modulator  
Authors : Staker, B.L.; Burgin Jr., A.B.  
Deposited on : 2009-07-13  
Resolution : 2.65 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

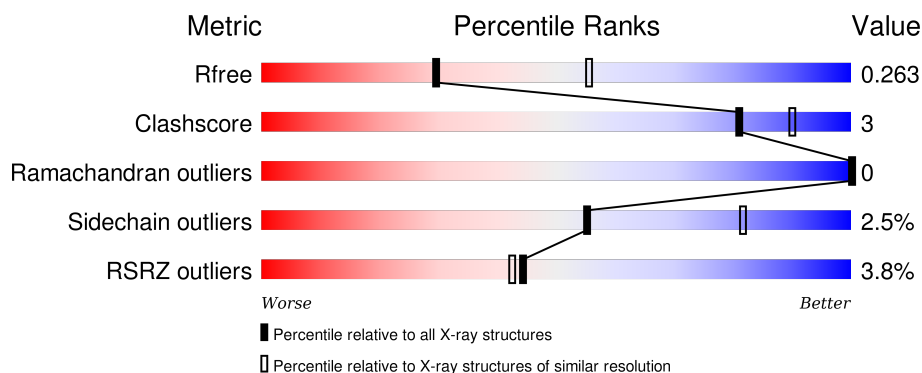
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	377	<div> <div>5%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>
1	B	377	<div> <div>2%</div> <div>81%</div> <div>9%</div> <div>10%</div> </div>
1	C	377	<div> <div>5%</div> <div>81%</div> <div>9%</div> <div>10%</div> </div>
1	D	377	<div> <div>2%</div> <div>83%</div> <div>6%</div> <div>10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	15X	B	901[A]	-	-	-	X
2	15X	B	901[B]	-	-	-	X
4	MG	A	621	-	-	-	X
5	EPE	A	806	-	-	-	X
5	EPE	D	804	-	-	-	X
5	EPE	D	805	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11397 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2743	1734	465	530	14			
1	B	338	Total	C	N	O	S	0	0	0
			2727	1726	462	525	14			
1	C	339	Total	C	N	O	S	0	0	0
			2740	1732	466	528	14			
1	D	339	Total	C	N	O	S	0	0	0
			2741	1733	467	527	14			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	INITIATING METHIONINE	UNP Q08499
A	579	ALA	-	LINKER	UNP Q08499
A	580	PRO	-	LINKER	UNP Q08499
A	581	ALA	-	LINKER	UNP Q08499
A	582	PRO	-	LINKER	UNP Q08499
A	583	PRO	-	LINKER	UNP Q08499
A	584	LEU	-	LINKER	UNP Q08499
A	585	ASP	-	LINKER	UNP Q08499
A	586	GLU	-	LINKER	UNP Q08499
A	587	GLN	-	LINKER	UNP Q08499
A	588	ASN	-	LINKER	UNP Q08499
A	589	ARG	-	LINKER	UNP Q08499
A	590	ASP	-	LINKER	UNP Q08499
A	591	SER	-	LINKER	UNP Q08499
A	592	GLN	-	LINKER	UNP Q08499
A	607	GLU	-	EXPRESSION TAG	UNP Q08499
A	608	ASN	-	EXPRESSION TAG	UNP Q08499
A	609	LEU	-	EXPRESSION TAG	UNP Q08499
A	610	TYR	-	EXPRESSION TAG	UNP Q08499
A	611	PHE	-	EXPRESSION TAG	UNP Q08499
A	612	GLN	-	EXPRESSION TAG	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
A	613	GLY	-	EXPRESSION TAG	UNP Q08499
A	614	HIS	-	EXPRESSION TAG	UNP Q08499
A	615	HIS	-	EXPRESSION TAG	UNP Q08499
A	616	HIS	-	EXPRESSION TAG	UNP Q08499
A	617	HIS	-	EXPRESSION TAG	UNP Q08499
A	618	HIS	-	EXPRESSION TAG	UNP Q08499
A	619	HIS	-	EXPRESSION TAG	UNP Q08499
B	243	MET	-	INITIATING METHIONINE	UNP Q08499
B	579	ALA	-	LINKER	UNP Q08499
B	580	PRO	-	LINKER	UNP Q08499
B	581	ALA	-	LINKER	UNP Q08499
B	582	PRO	-	LINKER	UNP Q08499
B	583	PRO	-	LINKER	UNP Q08499
B	584	LEU	-	LINKER	UNP Q08499
B	585	ASP	-	LINKER	UNP Q08499
B	586	GLU	-	LINKER	UNP Q08499
B	587	GLN	-	LINKER	UNP Q08499
B	588	ASN	-	LINKER	UNP Q08499
B	589	ARG	-	LINKER	UNP Q08499
B	590	ASP	-	LINKER	UNP Q08499
B	591	SER	-	LINKER	UNP Q08499
B	592	GLN	-	LINKER	UNP Q08499
B	607	GLU	-	EXPRESSION TAG	UNP Q08499
B	608	ASN	-	EXPRESSION TAG	UNP Q08499
B	609	LEU	-	EXPRESSION TAG	UNP Q08499
B	610	TYR	-	EXPRESSION TAG	UNP Q08499
B	611	PHE	-	EXPRESSION TAG	UNP Q08499
B	612	GLN	-	EXPRESSION TAG	UNP Q08499
B	613	GLY	-	EXPRESSION TAG	UNP Q08499
B	614	HIS	-	EXPRESSION TAG	UNP Q08499
B	615	HIS	-	EXPRESSION TAG	UNP Q08499
B	616	HIS	-	EXPRESSION TAG	UNP Q08499
B	617	HIS	-	EXPRESSION TAG	UNP Q08499
B	618	HIS	-	EXPRESSION TAG	UNP Q08499
B	619	HIS	-	EXPRESSION TAG	UNP Q08499
C	243	MET	-	INITIATING METHIONINE	UNP Q08499
C	579	ALA	-	LINKER	UNP Q08499
C	580	PRO	-	LINKER	UNP Q08499
C	581	ALA	-	LINKER	UNP Q08499
C	582	PRO	-	LINKER	UNP Q08499
C	583	PRO	-	LINKER	UNP Q08499
C	584	LEU	-	LINKER	UNP Q08499

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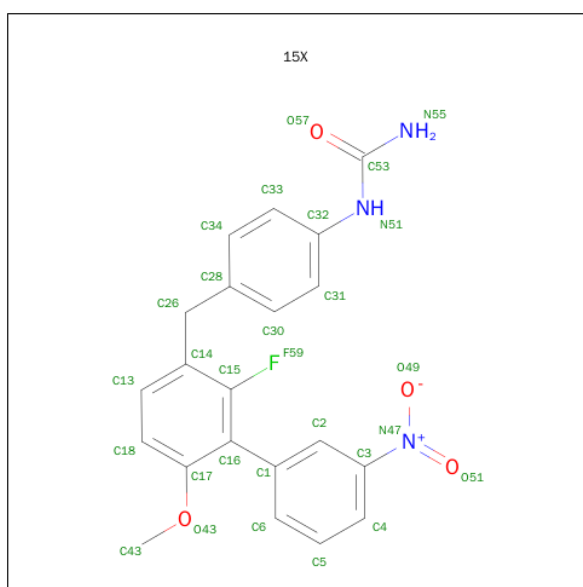
Chain	Residue	Modelled	Actual	Comment	Reference
C	585	ASP	-	LINKER	UNP Q08499
C	586	GLU	-	LINKER	UNP Q08499
C	587	GLN	-	LINKER	UNP Q08499
C	588	ASN	-	LINKER	UNP Q08499
C	589	ARG	-	LINKER	UNP Q08499
C	590	ASP	-	LINKER	UNP Q08499
C	591	SER	-	LINKER	UNP Q08499
C	592	GLN	-	LINKER	UNP Q08499
C	607	GLU	-	EXPRESSION TAG	UNP Q08499
C	608	ASN	-	EXPRESSION TAG	UNP Q08499
C	609	LEU	-	EXPRESSION TAG	UNP Q08499
C	610	TYR	-	EXPRESSION TAG	UNP Q08499
C	611	PHE	-	EXPRESSION TAG	UNP Q08499
C	612	GLN	-	EXPRESSION TAG	UNP Q08499
C	613	GLY	-	EXPRESSION TAG	UNP Q08499
C	614	HIS	-	EXPRESSION TAG	UNP Q08499
C	615	HIS	-	EXPRESSION TAG	UNP Q08499
C	616	HIS	-	EXPRESSION TAG	UNP Q08499
C	617	HIS	-	EXPRESSION TAG	UNP Q08499
C	618	HIS	-	EXPRESSION TAG	UNP Q08499
C	619	HIS	-	EXPRESSION TAG	UNP Q08499
D	243	MET	-	INITIATING METHIONINE	UNP Q08499
D	579	ALA	-	LINKER	UNP Q08499
D	580	PRO	-	LINKER	UNP Q08499
D	581	ALA	-	LINKER	UNP Q08499
D	582	PRO	-	LINKER	UNP Q08499
D	583	PRO	-	LINKER	UNP Q08499
D	584	LEU	-	LINKER	UNP Q08499
D	585	ASP	-	LINKER	UNP Q08499
D	586	GLU	-	LINKER	UNP Q08499
D	587	GLN	-	LINKER	UNP Q08499
D	588	ASN	-	LINKER	UNP Q08499
D	589	ARG	-	LINKER	UNP Q08499
D	590	ASP	-	LINKER	UNP Q08499
D	591	SER	-	LINKER	UNP Q08499
D	592	GLN	-	LINKER	UNP Q08499
D	607	GLU	-	EXPRESSION TAG	UNP Q08499
D	608	ASN	-	EXPRESSION TAG	UNP Q08499
D	609	LEU	-	EXPRESSION TAG	UNP Q08499
D	610	TYR	-	EXPRESSION TAG	UNP Q08499
D	611	PHE	-	EXPRESSION TAG	UNP Q08499
D	612	GLN	-	EXPRESSION TAG	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
D	613	GLY	-	EXPRESSION TAG	UNP Q08499
D	614	HIS	-	EXPRESSION TAG	UNP Q08499
D	615	HIS	-	EXPRESSION TAG	UNP Q08499
D	616	HIS	-	EXPRESSION TAG	UNP Q08499
D	617	HIS	-	EXPRESSION TAG	UNP Q08499
D	618	HIS	-	EXPRESSION TAG	UNP Q08499
D	619	HIS	-	EXPRESSION TAG	UNP Q08499

- Molecule 2 is 1-{4-[(2-FLUORO-6-METHOXY-3'-NITROBIPHENYL-3-YL)METHYL]PHENYL}UREA (three-letter code: 15X) (formula: C<sub>21</sub>H<sub>18</sub>FN<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 29	C 21	F 1	N 3	O 4	0	0
2	B	1	Total 58	C 42	F 2	N 6	O 8	0	1
2	C	1	Total 29	C 21	F 1	N 3	O 4	0	0
2	D	1	Total 29	C 21	F 1	N 3	O 4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

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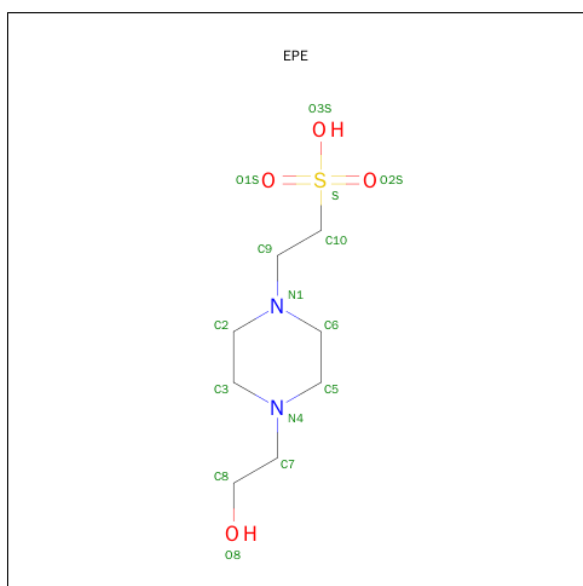
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

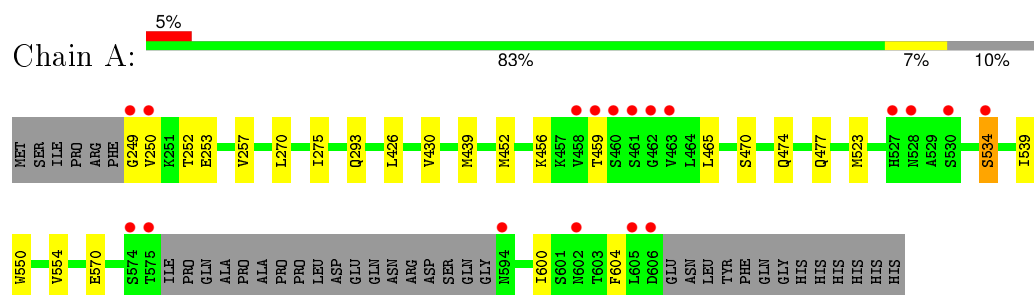
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	53	Total	O	0	0
			53	53		
6	B	46	Total	O	0	0
			46	46		
6	C	44	Total	O	0	0
			44	44		
6	D	60	Total	O	0	0
			60	60		

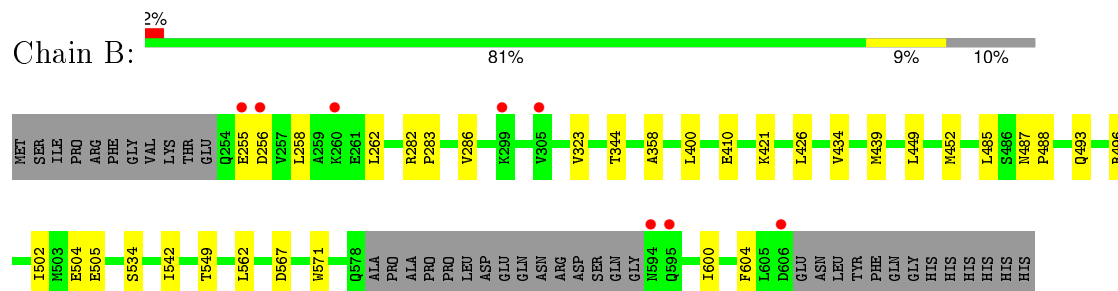
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

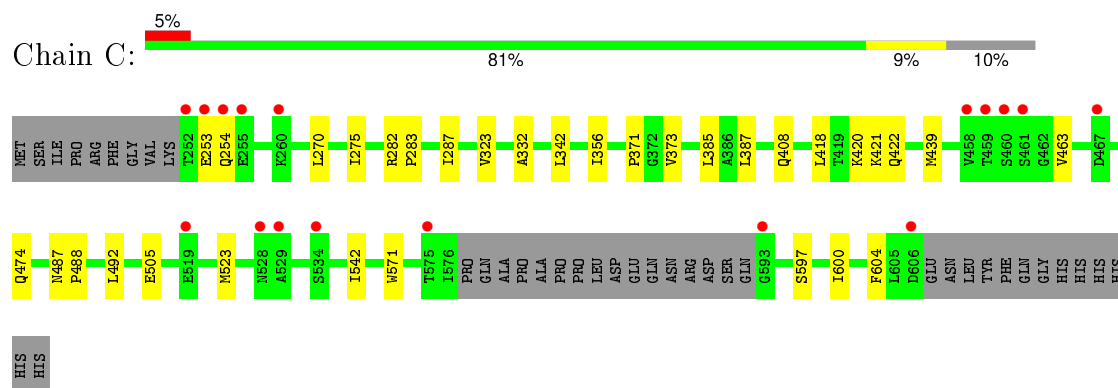
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



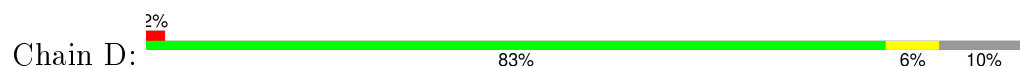
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

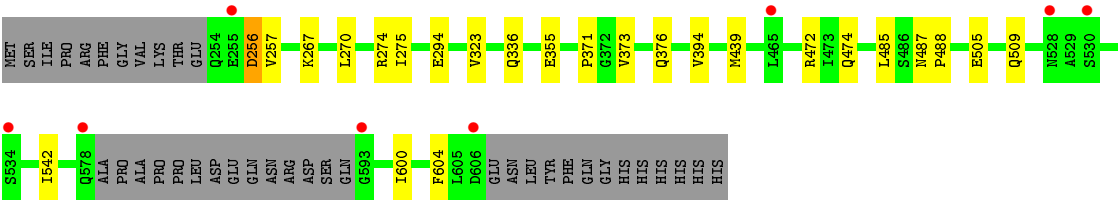


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.55Å 112.00Å 162.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 48.78 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.65) 93.2 (48.78-2.65)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.214 , 0.267 0.214 , 0.263	Depositor DCC
$R_{free}$ test set	2472 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 40.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 48954 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 15X, ZN, EPE, MG

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	0.35	0/2797	0.48	0/3798
1	B	0.35	0/2782	0.49	0/3780
1	C	0.36	0/2794	0.49	0/3794
1	D	0.37	0/2796	0.51	0/3797
All	All	0.36	0/11169	0.49	0/15169

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2743	0	2682	17	0
1	B	2727	0	2664	17	0
1	C	2740	0	2682	15	0
1	D	2741	0	2684	17	0
2	A	29	0	18	1	0
2	B	58	0	36	6	0
2	C	29	0	18	1	0
2	D	29	0	18	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	15	0	17	0	0
5	B	30	0	34	0	0
5	C	15	0	17	0	0
5	D	30	0	34	0	0
6	A	53	0	0	3	0
6	B	46	0	0	0	0
6	C	44	0	0	0	0
6	D	60	0	0	2	0
All	All	11397	0	10904	73	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 3.

All (73) 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:A:542:ILE:HD11	1:A:600:ILE:HG23	1.54	0.86
1:C:542:ILE:HD11	1:C:600:ILE:HG23	1.59	0.84
1:D:439:MET:HE2	1:D:604:PHE:HE2	1.41	0.84
1:D:542:ILE:HD11	1:D:600:ILE:HG23	1.58	0.83
2:B:901[A]:15X:H31	2:B:901[A]:15X:O57	1.80	0.80
1:B:542:ILE:HD11	1:B:600:ILE:HG23	1.66	0.77
1:D:439:MET:HE2	1:D:604:PHE:CE2	2.22	0.74
2:B:901[B]:15X:O57	2:B:901[B]:15X:H33	1.90	0.70
1:B:439:MET:HE2	1:B:604:PHE:HE2	1.59	0.66
1:B:358:ALA:HB2	1:B:426:LEU:HD12	1.78	0.65
1:B:439:MET:HE2	1:B:604:PHE:CE2	2.32	0.64
1:A:270:LEU:HD11	1:A:275:ILE:HD11	1.86	0.58
1:C:270:LEU:HD11	1:C:275:ILE:HD11	1.85	0.57
1:A:459:THR:HG22	1:A:465:LEU:HD12	1.87	0.56
1:B:323:VAL:HG13	1:B:505:GLU:OE1	2.05	0.56
1:C:323:VAL:HG13	1:C:505:GLU:OE1	2.08	0.54
1:D:267:LYS:NZ	6:D:30:HOH:O	2.40	0.54
1:B:400:LEU:HD21	1:B:434:VAL:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HD13	1:A:604:PHE:CE1	2.45	0.52
1:C:323:VAL:CG1	1:C:505:GLU:OE1	2.58	0.52
1:B:496:ARG:HD3	1:B:571:TRP:CH2	2.44	0.52
1:D:270:LEU:HD11	1:D:275:ILE:HD11	1.90	0.52
1:C:418:LEU:HD23	1:C:422:GLN:HB3	1.91	0.52
1:A:550:TRP:O	1:A:554:VAL:HG22	2.10	0.51
1:C:439:MET:HE2	1:C:604:PHE:CE2	2.46	0.51
2:B:901[B]:15X:F59	2:B:901[B]:15X:H30	2.01	0.51
1:D:487:ASN:HB2	1:D:488:PRO:HD3	1.93	0.50
1:D:439:MET:HE1	1:D:485:LEU:HD21	1.95	0.49
1:A:474:GLN:HA	1:A:477:GLN:HE21	1.76	0.49
1:B:449:LEU:HG	1:B:549:THR:HG22	1.96	0.48
1:A:523:MET:SD	1:A:534:SER:OG	2.71	0.48
1:D:371:PRO:HG2	1:D:373:VAL:HG22	1.96	0.47
2:A:901:15X:HN55	2:A:901:15X:H31	1.80	0.47
1:C:542:ILE:HD13	1:C:604:PHE:CD1	2.50	0.47
1:C:287:ILE:HD12	1:C:332:ALA:HB1	1.96	0.47
1:B:262:LEU:HD11	1:B:286:VAL:CG1	2.45	0.47
1:D:394:VAL:HG23	6:D:47:HOH:O	2.15	0.46
1:D:439:MET:HE3	1:D:439:MET:HA	1.97	0.46
1:D:323:VAL:HG13	1:D:505:GLU:OE1	2.15	0.46
1:A:426:LEU:O	1:A:430:VAL:HG23	2.15	0.46
1:A:249:GLY:N	6:A:93:HOH:O	2.48	0.46
1:A:439:MET:HE2	1:A:604:PHE:CE2	2.50	0.46
1:D:256:ASP:OD2	1:D:257:VAL:HG23	2.15	0.46
2:B:901[A]:15X:C31	2:B:901[A]:15X:O57	2.48	0.46
1:B:439:MET:HA	1:B:439:MET:HE3	1.98	0.46
2:D:901:15X:O57	2:D:901:15X:H33	2.16	0.45
1:A:250:VAL:HG22	6:A:93:HOH:O	2.17	0.45
1:A:439:MET:HA	1:A:439:MET:HE3	1.98	0.45
1:D:373:VAL:HA	1:D:509:GLN:HE21	1.82	0.45
2:C:901:15X:H33	2:C:901:15X:O57	2.17	0.45
2:B:901[B]:15X:O57	2:B:901[B]:15X:C33	2.57	0.44
1:C:492:LEU:HD21	1:C:571:TRP:CE2	2.51	0.44
1:B:542:ILE:HD13	1:B:604:PHE:CE1	2.52	0.44
1:B:282:ARG:N	1:B:283:PRO:CD	2.81	0.44
1:C:487:ASN:HB2	1:C:488:PRO:HD3	2.00	0.43
1:A:439:MET:HE2	1:A:604:PHE:HE2	1.83	0.43
1:B:410:GLU:CD	1:C:420:LYS:HZ3	2.22	0.43
1:A:253:GLU:O	1:A:257:VAL:HG23	2.19	0.43
1:D:373:VAL:HA	1:D:509:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:N	1:C:283:PRO:CD	2.83	0.42
1:D:270:LEU:HD22	1:D:336:GLN:HG3	2.01	0.42
1:A:539:ILE:HA	1:A:543:VAL:HB	2.02	0.42
1:C:342:LEU:HD13	1:C:356:ILE:HG23	2.01	0.42
1:C:371:PRO:HG2	1:C:373:VAL:HG22	2.02	0.41
1:A:293:GLN:NE2	6:A:87:HOH:O	2.51	0.41
1:D:542:ILE:HD13	1:D:604:PHE:CE1	2.56	0.41
1:B:502:ILE:HG21	2:B:901[A]:15X:H43A	2.01	0.41
1:C:439:MET:HA	1:C:439:MET:HE3	2.02	0.41
1:B:439:MET:HE1	1:B:485:LEU:HD21	2.02	0.41
1:D:355:GLU:OE1	1:D:472:ARG:NH1	2.54	0.41
1:B:487:ASN:HB2	1:B:488:PRO:HD3	2.03	0.41
1:A:459:THR:HG23	1:A:465:LEU:HB2	2.04	0.40
1:B:562:LEU:HA	1:B:562:LEU:HD23	1.97	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	336/377 (89%)	326 (97%)	10 (3%)	0	100	100
1	B	334/377 (89%)	321 (96%)	13 (4%)	0	100	100
1	C	335/377 (89%)	325 (97%)	10 (3%)	0	100	100
1	D	335/377 (89%)	327 (98%)	8 (2%)	0	100	100
All	All	1340/1508 (89%)	1299 (97%)	41 (3%)	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	310/344 (90%)	304 (98%)	6 (2%)	65	87
1	B	308/344 (90%)	298 (97%)	10 (3%)	46	74
1	C	310/344 (90%)	300 (97%)	10 (3%)	46	74
1	D	310/344 (90%)	305 (98%)	5 (2%)	70	89
All	All	1238/1376 (90%)	1207 (98%)	31 (2%)	55	82

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	THR
1	A	452	MET
1	A	456	LYS
1	A	470	SER
1	A	534	SER
1	A	570	GLU
1	B	255	GLU
1	B	256	ASP
1	B	258	LEU
1	B	344	THR
1	B	421	LYS
1	B	452	MET
1	B	493	GLN
1	B	504	GLU
1	B	534	SER
1	B	567	ASP
1	C	253	GLU
1	C	254	GLN
1	C	385	LEU
1	C	387	LEU
1	C	408	GLN
1	C	421	LYS
1	C	463	VAL
1	C	474	GLN

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Mol	Chain	Res	Type
1	C	523	MET
1	C	597	SER
1	D	256	ASP
1	D	274	ARG
1	D	294	GLU
1	D	376	GLN
1	D	474	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	477	GLN
1	A	528	ASN
1	D	254	GLN
1	D	293	GLN
1	D	416	GLN
1	D	509	GLN
1	D	528	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	$\# Z  > 2$
5	EPE	A	806	-	14,15,15	0.33	0	18,20,20	1.39	3 (16%)
2	15X	A	901	-	29,31,31	2.90	5 (17%)	39,43,43	2.59	11 (28%)
5	EPE	B	801	-	14,15,15	0.34	0	18,20,20	1.28	2 (11%)
5	EPE	B	802	-	14,15,15	0.38	0	18,20,20	1.37	2 (11%)
2	15X	B	901[A]	-	29,31,31	2.78	5 (17%)	39,43,43	1.67	9 (23%)
2	15X	B	901[B]	-	29,31,31	2.79	5 (17%)	39,43,43	1.59	8 (20%)
5	EPE	C	803	-	14,15,15	0.32	0	18,20,20	1.78	3 (16%)
2	15X	C	901	-	29,31,31	2.73	5 (17%)	39,43,43	1.91	10 (25%)
5	EPE	D	804	-	14,15,15	0.32	0	18,20,20	1.56	2 (11%)
5	EPE	D	805	-	14,15,15	0.37	0	18,20,20	1.80	2 (11%)
2	15X	D	901	-	29,31,31	2.67	5 (17%)	39,43,43	1.57	8 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	A	806	-	-	0/9/19/19	0/1/1/1
2	15X	A	901	-	-	2/18/18/18	0/3/3/3
5	EPE	B	801	-	-	0/9/19/19	0/1/1/1
5	EPE	B	802	-	-	0/9/19/19	0/1/1/1
2	15X	B	901[A]	-	-	0/18/18/18	0/3/3/3
2	15X	B	901[B]	-	-	0/18/18/18	0/3/3/3
5	EPE	C	803	-	-	0/9/19/19	0/1/1/1
2	15X	C	901	-	-	0/18/18/18	0/3/3/3
5	EPE	D	804	-	-	0/9/19/19	0/1/1/1
5	EPE	D	805	-	-	0/9/19/19	0/1/1/1
2	15X	D	901	-	-	0/18/18/18	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901[A]	15X	C32-N51	-2.93	1.36	1.41
2	B	901[B]	15X	C32-N51	-2.74	1.36	1.41
2	D	901	15X	C32-N51	-2.39	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	15X	C32-N51	-2.34	1.37	1.41
2	C	901	15X	C32-N51	-2.20	1.37	1.41
2	B	901[A]	15X	C16-C15	4.93	1.47	1.39
2	B	901[B]	15X	C16-C15	4.96	1.48	1.39
2	C	901	15X	C16-C15	4.98	1.48	1.39
2	D	901	15X	C16-C15	5.08	1.48	1.39
2	A	901	15X	C16-C15	5.18	1.48	1.39
2	D	901	15X	C16-C17	5.56	1.48	1.40
2	A	901	15X	C16-C17	5.78	1.48	1.40
2	B	901[A]	15X	C16-C17	5.89	1.48	1.40
2	B	901[B]	15X	C16-C17	5.89	1.48	1.40
2	C	901	15X	C16-C17	6.22	1.49	1.40
2	C	901	15X	C14-C15	8.14	1.47	1.38
2	D	901	15X	C14-C15	8.29	1.47	1.38
2	D	901	15X	O51-N47	8.30	1.39	1.22
2	B	901[A]	15X	O51-N47	8.49	1.39	1.22
2	B	901[B]	15X	O51-N47	8.50	1.39	1.22
2	C	901	15X	O51-N47	8.65	1.39	1.22
2	B	901[A]	15X	C14-C15	8.70	1.47	1.38
2	A	901	15X	O51-N47	8.80	1.40	1.22
2	B	901[B]	15X	C14-C15	8.87	1.48	1.38
2	A	901	15X	C14-C15	9.64	1.49	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	15X	O57-C53-N51	-5.68	115.42	122.72
2	C	901	15X	C1-C16-C15	-3.95	116.22	122.27
2	A	901	15X	O57-C53-N55	-3.81	116.77	123.30
2	A	901	15X	C1-C16-C15	-3.33	117.17	122.27
2	D	901	15X	O57-C53-N55	-3.26	117.72	123.30
2	C	901	15X	O57-C53-N55	-3.07	118.04	123.30
2	B	901[A]	15X	C1-C16-C15	-2.85	117.90	122.27
2	B	901[B]	15X	C1-C16-C15	-2.72	118.10	122.27
2	B	901[A]	15X	O43-C17-C18	-2.67	119.86	124.35
2	D	901	15X	C1-C16-C15	-2.66	118.20	122.27
2	B	901[B]	15X	O43-C17-C18	-2.61	119.95	124.35
2	B	901[A]	15X	C14-C26-C28	-2.55	108.04	114.04
2	C	901	15X	C26-C14-C15	-2.39	118.25	123.17
2	B	901[A]	15X	C26-C14-C15	-2.27	118.49	123.17
2	C	901	15X	O43-C17-C18	-2.24	120.59	124.35
2	B	901[B]	15X	O57-C53-N55	-2.23	119.47	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	15X	C26-C14-C15	-2.19	118.66	123.17
5	A	806	EPE	O2S-S-C10	2.02	108.63	106.91
2	B	901[A]	15X	N55-C53-N51	2.03	117.55	115.02
2	A	901	15X	C4-C3-N47	2.12	121.19	119.48
5	A	806	EPE	C6-N1-C2	2.12	113.50	108.90
2	A	901	15X	C31-C32-N51	2.13	127.53	120.41
2	B	901[B]	15X	N55-C53-N51	2.13	117.67	115.02
2	D	901	15X	O43-C17-C16	2.21	118.66	115.38
5	C	803	EPE	C6-C5-N4	2.25	114.66	110.63
2	D	901	15X	F59-C15-C14	2.31	120.00	117.75
5	B	801	EPE	O1S-S-C10	2.35	108.91	106.91
2	C	901	15X	F59-C15-C14	2.42	120.10	117.75
2	A	901	15X	O43-C17-C16	2.45	119.00	115.38
2	C	901	15X	C43-O43-C17	2.53	121.37	117.54
2	D	901	15X	C1-C16-C17	2.62	123.34	120.81
5	D	804	EPE	O1S-S-C10	2.69	109.20	106.91
2	B	901[B]	15X	C1-C16-C17	2.93	123.64	120.81
5	B	802	EPE	O2S-S-C10	3.07	109.53	106.91
2	B	901[A]	15X	F59-C15-C14	3.07	120.74	117.75
2	A	901	15X	C43-O43-C17	3.15	122.32	117.54
5	B	801	EPE	O2S-S-C10	3.17	109.61	106.91
2	C	901	15X	C4-C3-N47	3.20	122.07	119.48
2	B	901[B]	15X	F59-C15-C14	3.27	120.93	117.75
2	B	901[A]	15X	C1-C16-C17	3.35	124.05	120.81
2	D	901	15X	C43-O43-C17	3.41	122.71	117.54
2	A	901	15X	C1-C16-C17	3.45	124.15	120.81
5	D	805	EPE	O1S-S-C10	3.52	109.91	106.91
2	A	901	15X	C13-C14-C15	3.59	118.55	116.42
2	B	901[A]	15X	O43-C17-C16	3.69	120.84	115.38
2	C	901	15X	O43-C17-C16	3.71	120.86	115.38
2	B	901[B]	15X	O43-C17-C16	3.71	120.86	115.38
5	A	806	EPE	O1S-S-C10	3.83	110.17	106.91
2	D	901	15X	C13-C14-C15	4.11	118.86	116.42
5	B	802	EPE	O1S-S-C10	4.17	110.46	106.91
5	C	803	EPE	O1S-S-C10	4.37	110.63	106.91
2	A	901	15X	F59-C15-C14	4.43	122.06	117.75
2	C	901	15X	C13-C14-C15	4.54	119.12	116.42
2	B	901[B]	15X	C13-C14-C15	4.61	119.15	116.42
5	C	803	EPE	O2S-S-C10	4.63	110.86	106.91
2	B	901[A]	15X	C13-C14-C15	4.82	119.28	116.42
2	C	901	15X	C1-C16-C17	4.88	125.53	120.81
5	D	804	EPE	O2S-S-C10	5.20	111.34	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	805	EPE	O2S-S-C10	5.25	111.38	106.91
2	A	901	15X	N55-C53-N51	10.27	127.80	115.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	15X	O57-C53-N51-C32
2	A	901	15X	N55-C53-N51-C32

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	15X	1	0
2	B	901[A]	15X	3	0
2	B	901[B]	15X	3	0
2	C	901	15X	1	0
2	D	901	15X	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	340/377 (90%)	0.27	19 (5%) 28 25	7, 19, 40, 51	0
1	B	338/377 (89%)	0.18	8 (2%) 62 60	8, 24, 38, 53	0
1	C	339/377 (89%)	0.29	17 (5%) 32 30	10, 23, 43, 56	0
1	D	339/377 (89%)	0.01	8 (2%) 62 60	6, 14, 32, 41	0
All	All	1356/1508 (89%)	0.19	52 (3%) 44 42	6, 20, 39, 56	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	SER	5.6
1	D	593	GLY	5.0
1	A	461	SER	5.0
1	C	593	GLY	4.8
1	C	253	GLU	4.7
1	A	249	GLY	4.1
1	C	254	GLN	3.8
1	A	458	VAL	3.8
1	A	594	ASN	3.7
1	C	252	THR	3.5
1	A	606	ASP	3.5
1	B	606	ASP	3.5
1	C	575	THR	3.5
1	A	463	VAL	3.4
1	C	460	SER	3.2
1	B	256	ASP	3.1
1	A	462	GLY	2.9
1	C	458	VAL	2.9
1	C	459	THR	2.9
1	B	594	ASN	2.8
1	A	459	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	528	ASN	2.8
1	D	530	SER	2.8
1	C	467	ASP	2.8
1	B	255	GLU	2.7
1	A	250	VAL	2.6
1	D	528	ASN	2.6
1	C	528	ASN	2.6
1	D	606	ASP	2.6
1	B	299	LYS	2.5
1	B	260	LYS	2.5
1	C	534	SER	2.5
1	D	578	GLN	2.5
1	A	605	LEU	2.4
1	B	595	GLN	2.4
1	C	461	SER	2.4
1	C	606	ASP	2.3
1	A	574	SER	2.3
1	A	527	HIS	2.3
1	D	534	SER	2.2
1	B	305	VAL	2.2
1	A	534	SER	2.2
1	C	260	LYS	2.2
1	C	255	GLU	2.2
1	C	519	GLU	2.2
1	D	255	GLU	2.2
1	D	465	LEU	2.1
1	A	530	SER	2.1
1	A	602	ASN	2.1
1	A	575	THR	2.1
1	A	541	TYR	2.1
1	C	529	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EPE	D	805	15/15	0.94	0.28	8.24	34,41,44,45	0
4	MG	A	621	1/1	0.89	0.22	6.45	17,17,17,17	0
5	EPE	A	806	15/15	0.91	0.32	4.33	52,57,58,59	0
5	EPE	D	804	15/15	0.93	0.24	3.49	41,43,43,44	0
2	15X	B	901[B]	29/29	0.90	0.27	2.56	13,14,16,16	29
2	15X	B	901[A]	29/29	0.90	0.27	2.38	19,20,21,21	29
5	EPE	C	803	15/15	0.96	0.23	1.81	31,33,37,37	0
2	15X	A	901	29/29	0.90	0.28	1.67	22,27,35,37	0
2	15X	D	901	29/29	0.93	0.24	1.37	16,19,26,27	0
2	15X	C	901	29/29	0.91	0.25	1.22	26,29,34,35	0
5	EPE	B	801	15/15	0.92	0.21	1.06	48,51,51,51	0
5	EPE	B	802	15/15	0.94	0.23	0.71	44,47,49,49	0
4	MG	B	621	1/1	0.95	0.14	-1.30	17,17,17,17	0
3	ZN	C	620	1/1	0.99	0.08	-4.59	16,16,16,16	0
3	ZN	B	620	1/1	0.99	0.08	-4.61	13,13,13,13	0
4	MG	C	621	1/1	0.97	0.06	-5.30	10,10,10,10	0
3	ZN	A	620	1/1	0.99	0.09	-6.33	14,14,14,14	0
3	ZN	D	620	1/1	1.00	0.08	-6.62	10,10,10,10	0
4	MG	D	621	1/1	0.97	0.06	-8.66	3,3,3,3	0

## 6.5 Other polymers

There are no such residues in this entry.