



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:06 AM GMT

PDB ID : 2PCE
Title : Crystal structure of putative mandelate racemase/muconate lactonizing enzyme from *Roseovarius nubinhibens* ISM
Authors : Bonanno, J.B.; Rutter, M.; Bain, K.T.; Lau, C.; Ozyurt, S.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-03-29
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

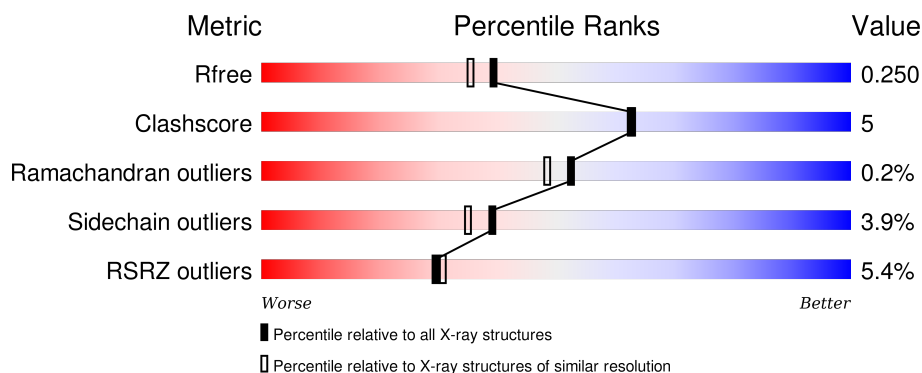
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 ≥ 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	386	
1	B	386	
1	C	386	
1	D	386	
1	E	386	

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Mol	Chain	Length	Quality of chain
1	F	386	
1	G	386	
1	H	386	

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	PO4	A	401	-	-	-	X
2	PO4	F	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23281 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 mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	4	0
			2796	1741	514	525	16			
1	B	371	Total	C	N	O	S	0	2	0
			2770	1724	507	523	16			
1	C	372	Total	C	N	O	S	0	1	0
			2777	1727	511	523	16			
1	D	372	Total	C	N	O	S	0	1	0
			2777	1727	511	523	16			
1	E	372	Total	C	N	O	S	0	1	0
			2777	1727	511	523	16			
1	F	370	Total	C	N	O	S	0	2	0
			2771	1725	510	520	16			
1	G	372	Total	C	N	O	S	0	3	0
			2788	1735	513	524	16			
1	H	372	Total	C	N	O	S	0	2	0
			2784	1732	513	523	16			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

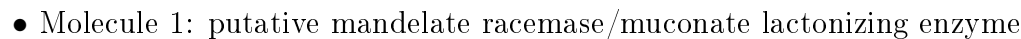
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		
3	B	111	Total	O	0	0
			111	111		
3	C	102	Total	O	0	0
			102	102		
3	D	128	Total	O	0	0
			128	128		


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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	143	Total 143	O 143	0	0
3	F	129	Total 129	O 129	0	0
3	G	114	Total 114	O 114	0	0
3	H	110	Total 110	O 110	0	0

- Molecule 1: putative mandelate racemase/muconate lactonizing enzyme



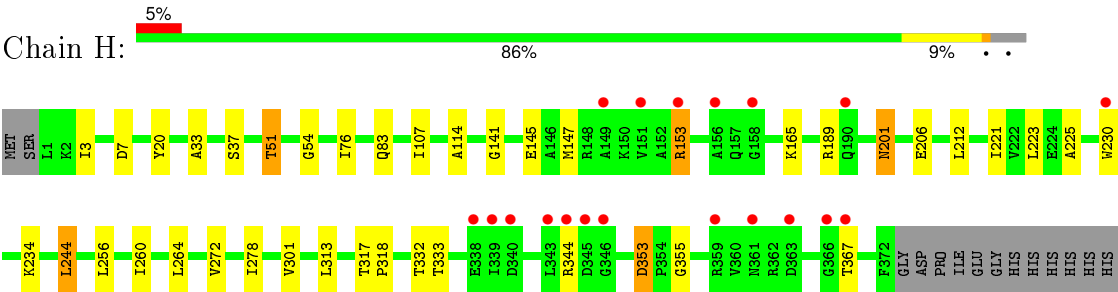
- Chain D: 

- Chain E:
-
- 86% 10% 4%
- Legend: MET, SER, L1, L6, T11, G18, V19, Y20, R21, E27, A33, T34, I35, V36, S37, I38, E39, T45, E49, S50, T51, G54, S55, P81, I87, L105, D106, I107, A114, L119, A146, P147, R148, A149, G158, K165, R181, A184, A187, D188

- Chain F:
-
- Sequence logo for Chain F, showing amino acid conservation across 300 positions. The y-axis represents information content in bits (0.00 to 0.10). The x-axis shows positions 1 to 300. A bar at the top indicates the percentage of conserved residues: 11% (red), 81% (green), and 14% (yellow).
- Key residues (positions and amino acids) are highlighted in the sequence logo:
- Position 1: MET
 - Position 2: SER
 - Position 3: L1
 - Position 4: I8
 - Position 5: V19
 - Position 6: Y20
 - Position 7: R21
 - Position 8: L22
 - Position 9: S23
 - Position 10: E27
 - Position 11: Y28
 - Position 12: A33
 - Position 13: V36
 - Position 14: S37
 - Position 15: W47
 - Position 16: T51
 - Position 17: P52
 - Position 18: F53
 - Position 19: G54
 - Position 20: L69
 - Position 21: Q63
 - Position 22: K96
 - Position 23: R99
 - Position 24: I107
 - Position 25: G118
 - Position 26: V135
 - Position 27: I136
 - Position 28: S137
 - Position 29: S138
 - Position 30: I139
 - Position 31: T143
 - Position 32: P144
 - Position 33: A145
 - Position 34: A146
 - Position 35: M147
 - Position 36: R148
 - Position 37: A149
 - Position 38: K150
 - Position 39: V151
 - Position 40: A152
 - Position 41: R153
 - Position 42: A156
 - Position 43: GLN
 - Position 44: GLY
 - Position 45: V201
 - Position 46: V204
 - Position 47: V207
 - Position 48: V210
 - Position 49: V213
 - Position 50: V216
 - Position 51: V219
 - Position 52: V222
 - Position 53: V225
 - Position 54: V228
 - Position 55: V231
 - Position 56: V234
 - Position 57: V237
 - Position 58: V240
 - Position 59: V243
 - Position 60: V246
 - Position 61: V249
 - Position 62: V252
 - Position 63: V255
 - Position 64: V258
 - Position 65: V261
 - Position 66: V264
 - Position 67: V267
 - Position 68: V270
 - Position 69: V273
 - Position 70: V276
 - Position 71: V279
 - Position 72: V282
 - Position 73: V285
 - Position 74: V288
 - Position 75: V291
 - Position 76: V294
 - Position 77: V297
 - Position 78: V300

- Chain G:
-
- Sequence logo for Chain G. The y-axis represents information content in bits (0.00 to 0.20). The x-axis lists amino acids. A color scale at the top indicates conservation levels: 2% (red), 81% (green), and 15% (yellow).
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1 | Met | 0.00 |
| 2 | Ser | 0.00 |
| 3 | Lys | 0.00 |
| 4 | Asp | 0.00 |
| 5 | Pro | 0.00 |
| 6 | Ile | 0.00 |
| 7 | Asn | 0.00 |
| 8 | Thr | 0.00 |
| 9 | Val | 0.00 |
| 10 | Leu | 0.00 |
| 11 | Ala | 0.00 |
| 12 | Arg | 0.00 |
| 13 | His | 0.00 |
| 14 | Pro | 0.00 |
| 15 | Leu | 0.00 |
| 16 | Val | 0.00 |
| 17 | Ala | 0.00 |
| 18 | Arg | 0.00 |
| 19 | His | 0.00 |
| 20 | Pro | 0.00 |
| 21 | Leu | 0.00 |
| 22 | Val | 0.00 |
| 23 | Ala | 0.00 |
| 24 | Arg | 0.00 |
| 25 | His | 0.00 |
| 26 | Pro | 0.00 |
| 27 | Leu | 0.00 |
| 28 | Val | 0.00 |
| 29 | Ala | 0.00 |
| 30 | Arg | 0.00 |
| 31 | His | 0.00 |
| 32 | Pro | 0.00 |
| 33 | Leu | 0.00 |
| 34 | Val | 0.00 |
| 35 | Ala | 0.00 |
| 36 | Arg | 0.00 |
| 37 | His | 0.00 |
| 38 | Pro | 0.00 |
| 39 | Leu | 0.00 |
| 40 | Val | 0.00 |
| 41 | Ala | 0.00 |
| 42 | Arg | 0.00 |
| 43 | His | 0.00 |
| 44 | Pro | 0.00 |
| 45 | Leu | 0.00 |
| 46 | Val | 0.00 |
| 47 | Ala | 0.00 |
| 48 | Arg | 0.00 |
| 49 | His | 0.00 |
| 50 | Pro | 0.00 |
| 51 | Leu | 0.00 |
| 52 | Val | 0.00 |
| 53 | Ala | 0.00 |
| 54 | Arg | 0.00 |
| 55 | His | 0.00 |
| 56 | Pro | 0.00 |
| 57 | Leu | 0.00 |
| 58 | Val | 0.00 |
| 59 | Ala | 0.00 |
| 60 | Arg | 0.00 |
| 61 | His | 0.00 |
| 62 | Pro | 0.00 |
| 63 | Leu | 0.00 |
| 64 | Val | 0.00 |
| 65 | Ala | 0.00 |
| 66 | Arg | 0.00 |
| 67 | His | 0.00 |
| 68 | Pro | 0.00 |
| 69 | Leu | 0.00 |
| 70 | Val | 0.00 |
| 71 | Ala | 0.00 |
| 72 | Arg | 0.00 |
| 73 | His | 0.00 |
| 74 | Pro | 0.00 |
| 75 | Leu | 0.00 |
| 76 | Val | 0.00 |
| 77 | Ala | 0.00 |
| 78 | Arg | 0.00 |
| 79 | His | 0.00 |
| 80 | Pro | 0.00 |
| 81 | Leu | 0.00 |
| 82 | Val | 0.00 |
| 83 | Ala | 0.00 |
| 84 | Arg | 0.00 |
| 85 | His | 0.00 |
| 86 | Pro | 0.00 |
| 87 | Leu | 0.00 |
| 88 | Val | 0.00 |
| 89 | Ala | 0.00 |
| 90 | Arg | 0.00 |
| 91 | His | 0.00 |
| 92 | Pro | 0.00 |
| 93 | Leu | 0.00 |
| 94 | Val | 0.00 |
| 95 | Ala | 0.00 |
| 96 | Arg | 0.00 |
| 97 | His | 0.00 |
| 98 | Pro | 0.00 |
| 99 | Leu | 0.00 |
| 100 | Val | 0.00 |
| 101 | Ala | 0.00 |
| 102 | Arg | 0.00 |
| 103 | His | 0.00 |
| 104 | Pro | 0.00 |
| 105 | Leu | 0.00 |
| 106 | Val | 0.00 |
| 107 | Ala | 0.00 |
| 108 | Arg | 0.00 |
| 109 | His | 0.00 |
| 110 | Pro | 0.00 |
| 111 | Leu | 0.00 |
| 112 | Val | 0.00 |
| 113 | Ala | 0.00 |
| 114 | Arg | 0.00 |
| 115 | His | 0.00 |
| 116 | Pro | 0.00 |
| 117 | Leu | 0.00 |
| 118 | Val | 0.00 |
| 119 | Ala | 0.00 |
| 120 | Arg | 0.00 |
| 121 | His | 0.00 |
| 122 | Pro | 0.00 |
| 123 | Leu | 0.00 |
| 124 | Val | 0.00 |
| 125 | Ala | 0.00 |
| 126 | Arg | 0.00 |
| 127 | His | 0.00 |
| 128 | Pro | 0.00 |
| 129 | Leu | 0.00 |
| 130 | Val | 0.00 |
| 131 | Ala | 0.00 |
| 132 | Arg | 0.00 |
| 133 | His | 0.00 |
| 134 | Pro | 0.00 |
| 135 | Leu | 0.00 |
| 136 | Val | 0.00 |
| 137 | Ala | 0.00 |
| 138 | Arg | 0.00 |
| 139 | His | 0.00 |
| 140 | Pro | 0.00 |
| 141 | Leu | 0.00 |
| 142 | Val | 0.00 |
| 143 | Ala | 0.00 |
| 144 | Arg | 0.00 |
| 145 | His | 0.00 |
| 146 | Pro | 0.00 |
| 147 | Leu | 0.00</ |

- Molecule 1: putative mandelate racemase/muconate lactonizing enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	168.69Å 174.41Å 108.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 49.55 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.00) 97.0 (49.55-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.250 0.204 , 0.250	Depositor DCC
R_{free} test set	10459 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 208314 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23281	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 20.16 % 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 9.2445e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.78	0/2853	0.84	3/3877 (0.1%)
1	B	0.71	0/2822	0.79	2/3834 (0.1%)
1	C	0.64	0/2827	0.79	2/3841 (0.1%)
1	D	0.73	0/2827	0.82	3/3841 (0.1%)
1	E	0.74	0/2827	0.79	3/3841 (0.1%)
1	F	0.76	0/2824	0.80	1/3836 (0.0%)
1	G	0.69	0/2845	0.79	2/3866 (0.1%)
1	H	0.72	0/2838	0.83	1/3856 (0.0%)
All	All	0.72	0/22663	0.81	17/30792 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	8

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	239	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	E	55	SER	N-CA-C	6.65	128.95	111.00
1	C	55	SER	N-CA-C	-6.37	93.81	111.00
1	B	239	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	E	55	SER	N-CA-CB	-6.04	101.44	110.50
1	G	239	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	196	LEU	CA-CB-CG	5.57	128.10	115.30
1	C	99	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	H	189	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	D	55	SER	N-CA-CB	5.37	118.55	110.50
1	E	198	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	55	SER	N-CA-C	-5.21	96.94	111.00
1	G	239	ARG	CG-CD-NE	-5.19	100.90	111.80
1	A	239	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	F	196	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	93	ASP	CB-CG-OD1	-5.05	113.76	118.30
1	A	99	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	GLY	Peptide
1	B	54	GLY	Peptide
1	C	54	GLY	Peptide
1	D	54	GLY	Peptide
1	E	54	GLY	Peptide
1	F	54	GLY	Peptide
1	G	54	GLY	Peptide
1	H	54	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2796	0	2821	25	0
1	B	2770	0	2790	27	0
1	C	2777	0	2797	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2777	0	2797	34	0
1	E	2777	0	2797	26	0
1	F	2771	0	2792	38	0
1	G	2788	0	2811	31	0
1	H	2784	0	2804	26	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	164	0	0	4	0
3	B	111	0	0	2	0
3	C	102	0	0	2	0
3	D	128	0	0	3	0
3	E	143	0	0	4	0
3	F	129	0	0	1	0
3	G	114	0	0	0	0
3	H	110	0	0	0	0
All	All	23281	0	22409	238	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 5.

All (238) 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:E:147:MET:HE1	1:E:181:ARG:HB3	1.37	1.02
3:E:428:HOH:O	1:F:83:GLN:HG2	1.60	1.00
1:H:234:LYS:HG2	1:H:264:LEU:HD11	1.47	0.97
1:H:153:ARG:HH11	1:H:153:ARG:HG3	1.27	0.95
1:D:141:GLY:HA2	1:D:147:MET:CE	1.98	0.94
1:G:139:ILE:HD13	1:G:151:VAL:HG22	1.52	0.90
1:C:141:GLY:HA2	1:C:147:MET:CE	2.03	0.88
1:A:359:ARG:HH11	1:A:359:ARG:HG3	1.40	0.84
1:F:143:THR:O	1:F:147:MET:HG3	1.79	0.83
1:E:147:MET:HE1	1:E:181:ARG:CB	2.09	0.82
1:E:208:ALA:O	1:E:212:LEU:HD13	1.80	0.82
1:H:153:ARG:HH11	1:H:153:ARG:CG	1.93	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:HD22	1:C:224:GLU:HB2	1.63	0.80
1:B:155:ARG:NH1	1:B:188:ASP:O	2.14	0.79
1:G:139:ILE:CD1	1:G:151:VAL:HG22	2.13	0.78
1:G:139:ILE:HD13	1:G:151:VAL:CG2	2.14	0.78
1:G:176:ALA:O	1:G:180:GLU:HG3	1.85	0.76
1:D:142:ASP:H	1:D:147:MET:CE	1.98	0.76
1:G:33:ALA:HA	1:G:51:THR:HB	1.68	0.75
1:H:141:GLY:HA2	1:H:147:MET:HE3	1.68	0.74
1:D:33:ALA:HA	1:D:51:THR:HB	1.70	0.74
1:C:114:ALA:HB3	1:C:355:GLY:HA2	1.70	0.73
1:C:142:ASP:H	1:C:147:MET:CE	2.01	0.73
1:F:33:ALA:HA	1:F:51:THR:HB	1.69	0.73
1:C:142:ASP:H	1:C:147:MET:HE3	1.54	0.73
1:B:143:THR:HB	3:B:411:HOH:O	1.86	0.73
1:H:33:ALA:HA	1:H:51:THR:HB	1.71	0.73
1:F:153:ARG:HH11	1:F:153:ARG:HG3	1.55	0.72
1:D:142:ASP:H	1:D:147:MET:HE3	1.54	0.71
1:D:141:GLY:HA2	1:D:147:MET:HE2	1.74	0.70
1:E:196:LEU:HD22	1:E:224:GLU:HB2	1.75	0.69
1:E:196:LEU:HD13	1:E:224:GLU:OE1	1.93	0.69
1:C:234:LYS:HG2	1:C:264:LEU:HD13	1.75	0.68
1:H:234:LYS:HG2	1:H:264:LEU:CD1	2.22	0.68
1:G:299:ASP:HB2	1:G:310:ILE:HD11	1.76	0.67
3:C:437:HOH:O	1:H:83:GLN:HG2	1.95	0.66
1:E:320:HIS:HD2	3:E:465:HOH:O	1.76	0.66
1:B:33:ALA:HA	1:B:51:THR:HB	1.77	0.66
1:H:153:ARG:HG3	1:H:153:ARG:NH1	2.04	0.66
1:C:142:ASP:N	1:C:147:MET:HE3	2.11	0.66
1:A:299:ASP:HB2	1:A:310:ILE:HD11	1.79	0.64
1:A:359:ARG:HG3	1:A:359:ARG:NH1	2.05	0.64
1:G:196:LEU:HD13	1:G:224:GLU:OE1	1.99	0.63
1:B:114:ALA:HB3	1:B:355:GLY:HA2	1.80	0.63
1:F:196:LEU:HD22	1:F:224:GLU:HB2	1.80	0.63
1:C:226:PRO:HG3	1:C:244:LEU:HD11	1.82	0.62
1:E:33:ALA:HA	1:E:51:THR:HB	1.81	0.62
1:D:147:MET:HA	3:D:432:HOH:O	2.00	0.61
1:H:256:LEU:O	1:H:260:ILE:HD13	2.00	0.61
1:E:114:ALA:HB3	1:E:355:GLY:HA2	1.83	0.61
1:F:343:LEU:N	1:F:343:LEU:HD12	2.16	0.60
1:C:81:PRO:HA	1:C:87:ILE:HD11	1.82	0.60
1:B:155:ARG:HH11	1:B:190:GLN:HG2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:TYR:CE2	1:B:53:PHE:HE2	2.20	0.59
1:B:143:THR:CB	3:B:411:HOH:O	2.46	0.58
1:C:99:ARG:HD3	1:C:275:GLN:O	2.03	0.58
1:F:20:TYR:OH	1:F:165:LYS:HE3	2.03	0.58
1:G:114:ALA:HB3	1:G:355:GLY:HA2	1.84	0.58
1:C:8:ILE:CD1	1:C:372:PHE:HE2	2.16	0.58
1:B:28:TYR:CE2	1:B:53:PHE:CE2	2.91	0.58
1:C:141:GLY:HA2	1:C:147:MET:HE1	1.83	0.58
1:C:33:ALA:HA	1:C:51:THR:HB	1.85	0.57
1:F:189:ARG:NH2	1:F:193:GLU:O	2.37	0.57
1:A:141:GLY:HA2	1:A:147:MET:HE3	1.86	0.57
1:C:147:MET:HB3	1:C:185:CYS:SG	2.44	0.57
1:A:33:ALA:HA	1:A:51:THR:HB	1.87	0.57
1:G:307:PHE:HB2	1:G:328:THR:OG1	2.05	0.57
1:D:320:HIS:HD2	3:D:444:HOH:O	1.87	0.56
1:H:223:LEU:HB3	1:H:244:LEU:HD12	1.88	0.56
1:C:190:GLN:O	1:C:193:GLU:HG3	2.06	0.56
1:G:11:THR:HG22	1:G:35:ILE:CD1	2.35	0.56
1:A:47:TRP:CZ3	1:A:365:LEU:CD1	2.90	0.55
1:F:186:LEU:HD12	1:F:219:LEU:HD22	1.89	0.55
1:H:145:GLU:H	1:H:145:GLU:CD	2.09	0.54
1:F:164:ILE:O	1:F:164:ILE:HG13	2.07	0.54
1:H:230[A]:TRP:CD1	1:H:234:LYS:HE2	2.43	0.53
1:H:7:ASP:HB2	1:H:37:SER:OG	2.08	0.53
1:D:141:GLY:HA2	1:D:147:MET:HE1	1.89	0.53
1:G:20:TYR:OH	1:G:165:LYS:HE2	2.09	0.53
1:E:11:THR:HG22	1:E:35:ILE:CD1	2.39	0.53
1:D:201:ASN:HD22	1:D:225:ALA:HB1	1.73	0.53
1:F:136:ILE:HG23	1:F:137:SER:O	2.09	0.53
1:A:196[B]:LEU:HD11	1:A:224:GLU:HB2	1.91	0.53
1:F:8:ILE:HD13	1:F:36:VAL:HG22	1.91	0.52
1:C:55:SER:OG	1:G:94:THR:O	2.26	0.52
1:C:114:ALA:CB	1:C:355:GLY:HA2	2.38	0.52
1:B:196:LEU:HD22	1:B:224:GLU:HB2	1.90	0.52
1:F:194:TRP:CH2	1:F:196:LEU:HG	2.45	0.51
1:E:320:HIS:CD2	3:E:465:HOH:O	2.59	0.51
1:H:114:ALA:HB3	1:H:355:GLY:HA2	1.92	0.51
1:F:201:ASN:HD22	1:F:225:ALA:HB1	1.75	0.51
1:C:37:SER:HB3	1:C:47:TRP:CZ3	2.46	0.51
1:A:233:THR:HG21	1:A:246:LEU:HD21	1.93	0.50
1:F:147:MET:HB3	1:F:185:CYS:SG	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:VAL:O	1:F:325:ALA:HA	2.12	0.50
1:A:194:TRP:CZ3	1:A:196[A]:LEU:HG	2.47	0.50
1:D:37:SER:HB3	1:D:47:TRP:CZ3	2.46	0.50
1:D:142:ASP:H	1:D:147:MET:HE2	1.73	0.49
1:A:201:ASN:HD22	1:A:225:ALA:HB1	1.77	0.49
1:E:299:ASP:HB2	1:E:310:ILE:HD11	1.93	0.49
1:B:155:ARG:NH1	1:B:190:GLN:HG2	2.26	0.49
1:B:359:ARG:HH11	1:B:359:ARG:HG3	1.76	0.49
1:G:3:ILE:HG22	1:G:77:LEU:HD23	1.95	0.49
1:D:297:VAL:O	1:D:325:ALA:HA	2.13	0.49
1:A:230[B]:TRP:HD1	3:A:470:HOH:O	1.95	0.49
1:F:196:LEU:HD13	1:F:224:GLU:OE1	2.13	0.49
1:F:278:ILE:HG23	1:F:313:LEU:HD21	1.94	0.49
1:A:323:ARG:O	1:A:324:CYS:HB2	2.13	0.49
1:D:110:TRP:CD1	1:D:278:ILE:HB	2.48	0.49
1:F:323:ARG:O	1:F:324:CYS:HB2	2.13	0.49
1:A:133:VAL:HG13	1:A:322:LEU:HD21	1.95	0.49
1:F:107:ILE:HD11	1:F:272:VAL:CG1	2.43	0.49
1:A:20:TYR:OH	1:A:165:LYS:HE2	2.13	0.49
1:D:142:ASP:N	1:D:147:MET:CE	2.73	0.48
1:G:196:LEU:HD21	1:G:245:LEU:HD13	1.95	0.48
1:D:256:LEU:O	1:D:260:ILE:HD12	2.13	0.48
1:F:8:ILE:HD12	1:F:69:LEU:HD13	1.95	0.48
1:B:246:LEU:HG	1:B:265:CYS:HB3	1.95	0.48
1:G:370:LYS:HD2	1:G:371:THR:H	1.78	0.48
1:B:343:LEU:HA	1:B:347:GLY:O	2.14	0.48
1:D:142:ASP:N	1:D:147:MET:HE2	2.29	0.48
1:E:20:TYR:OH	1:E:165:LYS:HE2	2.13	0.48
1:B:135:VAL:HG23	1:B:159:PHE:CE1	2.49	0.48
1:F:37:SER:HB3	1:F:47:TRP:CZ3	2.48	0.48
1:F:153:ARG:HH11	1:F:153:ARG:CG	2.27	0.47
1:C:312:HIS:CE1	1:C:350:ALA:HB1	2.49	0.47
1:E:201:ASN:HD22	1:E:225:ALA:HB1	1.78	0.47
1:E:343:LEU:HD12	1:E:343:LEU:N	2.29	0.47
1:G:327:ASP:OD1	1:G:343:LEU:HD11	2.14	0.47
1:A:84[B]:HIS:HD2	3:A:461:HOH:O	1.97	0.47
1:B:196:LEU:CD2	1:B:224:GLU:HB2	2.43	0.47
1:G:110:TRP:CD1	1:G:278:ILE:HB	2.50	0.47
1:E:257:ILE:HD12	1:F:260:ILE:HD13	1.97	0.47
1:G:234:LYS:HE2	1:G:262:ASP:CG	2.35	0.46
1:D:222:VAL:HG22	1:D:243:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ILE:HD12	1:C:372:PHE:HE2	1.79	0.46
1:F:107:ILE:HD11	1:F:272:VAL:HG11	1.97	0.46
1:A:128:ARG:HD3	3:A:545:HOH:O	2.16	0.46
1:G:196:LEU:HD22	1:G:224:GLU:HB2	1.96	0.46
1:B:140:GLY:O	1:B:147:MET:HE3	2.16	0.46
1:D:234:LYS:HG2	1:D:264:LEU:HD13	1.96	0.46
1:E:49:GLU:OE2	1:E:51:THR:CG2	2.64	0.45
1:D:137:SER:OG	1:D:162:HIS:ND1	2.40	0.45
1:D:123:ASP:HA	1:D:127:GLY:HA2	1.97	0.45
1:C:196:LEU:HD13	1:C:224:GLU:OE1	2.16	0.45
1:B:162:HIS:CD2	1:B:195:TYR:CE2	3.04	0.45
1:B:37:SER:HB3	1:B:47:TRP:CZ3	2.52	0.45
1:F:135:VAL:HG23	1:F:159:PHE:CD1	2.51	0.45
1:B:99:ARG:HD3	1:B:275:GLN:O	2.15	0.45
1:D:338:GLU:HB2	1:D:359:ARG:HB2	1.97	0.45
1:D:169:SER:OG	1:D:172:GLU:HG3	2.16	0.45
1:G:13:LEU:HA	1:G:14:PRO:HD3	1.86	0.45
1:D:230[B]:TRP:HD1	3:D:441:HOH:O	1.99	0.45
1:H:20:TYR:OH	1:H:165:LYS:HE2	2.17	0.45
1:C:8:ILE:HD11	1:C:372:PHE:HE2	1.81	0.45
1:D:301:VAL:HG23	1:D:331:MET:HE2	2.00	0.44
1:H:353:ASP:N	1:H:353:ASP:OD2	2.50	0.44
1:A:114:ALA:HB3	1:A:355:GLY:HA2	1.99	0.44
1:G:19:VAL:HG22	1:G:29:HIS:CE1	2.52	0.44
1:C:153:ARG:O	1:C:157:GLN:HG3	2.17	0.44
1:E:21:ARG:HG2	1:E:27:GLU:HG2	1.99	0.44
1:G:37:SER:HB3	1:G:47:TRP:CZ3	2.52	0.44
1:A:47:TRP:CZ3	1:A:365:LEU:HD11	2.53	0.44
1:E:11:THR:HG22	1:E:35:ILE:HD11	2.00	0.44
1:C:216:PRO:HA	1:C:217:PRO:HD3	1.82	0.44
1:H:201:ASN:HD22	1:H:225:ALA:HB1	1.83	0.43
1:C:133:VAL:HG13	1:C:322:LEU:HD21	2.00	0.43
1:A:307:PHE:CE1	1:A:327:ASP:HA	2.53	0.43
1:F:213:SER:O	1:G:218:GLY:HA2	2.18	0.43
1:D:271:LYS:HA	1:D:298:GLN:O	2.18	0.43
1:H:153:ARG:NH1	1:H:153:ARG:CG	2.64	0.43
1:F:234:LYS:HG2	1:F:264:LEU:HD13	1.99	0.43
1:F:99:ARG:HD3	1:F:275:GLN:O	2.18	0.43
1:H:230[B]:TRP:O	1:H:234:LYS:HG3	2.19	0.43
1:C:137:SER:HB2	1:C:154:HIS:CD2	2.54	0.43
1:H:230[A]:TRP:CE2	1:H:264:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:GLY:CA	1:D:147:MET:HE2	2.45	0.43
1:D:359:ARG:HH11	1:D:359:ARG:HG3	1.84	0.43
1:E:6:ILE:HG12	1:E:38:ILE:HG12	1.99	0.43
1:C:141:GLY:HA2	1:C:147:MET:HE3	1.94	0.43
1:F:308:ALA:HB2	1:F:358:LEU:HD21	2.01	0.43
1:C:148:ARG:NH2	1:C:188:ASP:OD1	2.48	0.43
1:C:36:VAL:HG11	1:C:105:LEU:HD23	2.00	0.43
1:A:359:ARG:CG	1:A:359:ARG:HH11	2.18	0.43
1:B:297:VAL:O	1:B:325:ALA:HA	2.19	0.43
1:H:107:ILE:HD11	1:H:272:VAL:CG1	2.49	0.43
1:C:49:GLU:OE2	1:C:51:THR:CG2	2.67	0.42
1:B:3:ILE:HG13	1:B:81:PRO:HD3	2.00	0.42
1:G:223:LEU:HB3	1:G:244:LEU:HD12	2.01	0.42
1:E:344:ARG:HB3	1:E:344:ARG:HE	1.51	0.42
1:G:233:THR:HG21	1:G:246:LEU:HD21	2.00	0.42
1:C:220:ASP:HB2	1:D:214:LEU:HD21	2.00	0.42
1:E:49:GLU:OE2	1:E:51:THR:HG21	2.19	0.42
1:A:153:ARG:NH2	3:A:460:HOH:O	2.52	0.42
1:F:230[B]:TRP:HD1	3:F:420:HOH:O	2.02	0.42
1:C:142:ASP:N	1:C:147:MET:CE	2.75	0.42
1:B:359:ARG:HG3	1:B:359:ARG:NH1	2.35	0.42
1:D:36:VAL:HG11	1:D:105:LEU:HD23	2.00	0.42
1:H:278:ILE:HG23	1:H:313:LEU:HD21	2.00	0.42
1:C:194:TRP:CH2	1:C:196:LEU:HG	2.54	0.42
3:C:437:HOH:O	1:H:83:GLN:CG	2.61	0.42
1:H:3:ILE:HD13	1:H:76:ILE:HD12	2.00	0.42
1:E:107:ILE:HD11	1:E:272:VAL:CG1	2.49	0.42
1:B:147:MET:HB3	1:B:185:CYS:SG	2.60	0.42
1:F:28:TYR:CE2	1:F:53:PHE:HE2	2.38	0.42
1:B:22:LEU:HD22	1:B:200:ASN:OD1	2.20	0.42
1:G:11:THR:HG22	1:G:35:ILE:HD11	2.01	0.42
1:G:251:GLN:HG2	1:G:274:LYS:HG3	2.01	0.42
1:F:201:ASN:ND2	1:F:225:ALA:HB1	2.35	0.41
1:D:323:ARG:O	1:D:324:CYS:HB2	2.20	0.41
1:G:88:TRP:CD1	1:G:92:ARG:HD2	2.55	0.41
1:C:88:TRP:O	1:C:92:ARG:HG3	2.20	0.41
1:D:161:GLY:HA2	1:D:194:TRP:O	2.21	0.41
1:G:201:ASN:HD22	1:G:225:ALA:HB1	1.86	0.41
1:E:36:VAL:HG11	1:E:105:LEU:HD23	2.02	0.41
1:G:7:ASP:HB2	1:G:37:SER:OG	2.21	0.41
1:H:317:THR:HA	1:H:318:PRO:HD2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:ILE:O	1:F:165:LYS:HG2	2.20	0.41
1:A:110:TRP:CD1	1:A:278:ILE:HB	2.56	0.41
1:G:323:ARG:O	1:G:324:CYS:HB2	2.21	0.41
1:F:233:THR:HG21	1:F:246:LEU:HD21	2.02	0.41
1:C:169:SER:OG	1:C:172:GLU:HG3	2.21	0.41
1:B:31:TYR:CE1	1:B:301:VAL:HG21	2.55	0.41
1:F:343:LEU:CD1	1:F:343:LEU:N	2.83	0.41
1:A:20:TYR:HB3	1:A:28:TYR:HB2	2.02	0.41
1:B:9:HIS:CE1	1:B:368:PRO:HG3	2.56	0.41
1:A:234:LYS:HE2	1:A:262:ASP:OD1	2.21	0.41
1:F:8:ILE:CD1	1:F:36:VAL:HG22	2.50	0.41
1:A:299:ASP:CB	1:A:310:ILE:HD11	2.47	0.40
1:D:81:PRO:HA	1:D:87:ILE:HD11	2.03	0.40
1:F:196:LEU:HD22	1:F:224:GLU:CB	2.47	0.40
1:E:1:LEU:N	3:E:520:HOH:O	2.54	0.40
1:D:143:THR:O	1:D:147:MET:HG3	2.21	0.40
1:E:81:PRO:HA	1:E:87:ILE:HD11	2.03	0.40
1:H:230[A]:TRP:HD1	1:H:234:LYS:CE	2.34	0.40
1:B:194:TRP:CH2	1:B:196:LEU:HG	2.56	0.40
1:D:186:LEU:HD13	1:D:189:ARG:NH1	2.37	0.40
1:E:39:GLU:HG2	1:E:45:THR:OG1	2.21	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	374/386 (97%)	363 (97%)	10 (3%)	1 (0%)	46	41
1	B	369/386 (96%)	355 (96%)	13 (4%)	1 (0%)	46	41
1	C	371/386 (96%)	359 (97%)	11 (3%)	1 (0%)	46	41
1	D	371/386 (96%)	358 (96%)	12 (3%)	1 (0%)	46	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	371/386 (96%)	360 (97%)	11 (3%)	0	100	100
1	F	368/386 (95%)	351 (95%)	16 (4%)	1 (0%)	46	41
1	G	373/386 (97%)	362 (97%)	11 (3%)	0	100	100
1	H	372/386 (96%)	361 (97%)	10 (3%)	1 (0%)	46	41
All	All	2969/3088 (96%)	2869 (97%)	94 (3%)	6 (0%)	52	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	ASP
1	A	54	GLY
1	B	301	VAL
1	H	301	VAL
1	F	301	VAL
1	D	301	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/294 (97%)	270 (94%)	16 (6%)	26	20
1	B	283/294 (96%)	271 (96%)	12 (4%)	36	31
1	C	283/294 (96%)	274 (97%)	9 (3%)	46	44
1	D	283/294 (96%)	267 (94%)	16 (6%)	25	19
1	E	283/294 (96%)	279 (99%)	4 (1%)	74	77
1	F	283/294 (96%)	275 (97%)	8 (3%)	51	50
1	G	285/294 (97%)	275 (96%)	10 (4%)	43	40
1	H	284/294 (97%)	272 (96%)	12 (4%)	36	31
All	All	2270/2352 (96%)	2183 (96%)	87 (4%)	39	36

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	96	LYS
1	A	150	LYS
1	A	164	ILE
1	A	201	ASN
1	A	206	GLU
1	A	235	SER
1	A	239	ARG
1	A	244	LEU
1	A	306	SER
1	A	319	ARG
1	A	332	THR
1	A	333	THR
1	A	353	ASP
1	A	359	ARG
1	A	367	THR
1	B	51	THR
1	B	87	ILE
1	B	137	SER
1	B	142	ASP
1	B	188	ASP
1	B	196	LEU
1	B	201	ASN
1	B	206	GLU
1	B	212	LEU
1	B	333	THR
1	B	345	ASP
1	B	362	ARG
1	C	51	THR
1	C	96	LYS
1	C	201	ASN
1	C	212	LEU
1	C	332	THR
1	C	333	THR
1	C	344	ARG
1	C	365	LEU
1	C	367	THR
1	D	2	LYS
1	D	51	THR
1	D	137	SER
1	D	186	LEU
1	D	188	ASP
1	D	189	ARG

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Mol	Chain	Res	Type
1	D	201	ASN
1	D	206	GLU
1	D	212	LEU
1	D	239	ARG
1	D	242	LEU
1	D	244	LEU
1	D	332	THR
1	D	333	THR
1	D	343	LEU
1	D	344	ARG
1	E	51	THR
1	E	201	ASN
1	E	206	GLU
1	E	344	ARG
1	F	51	THR
1	F	96	LYS
1	F	153	ARG
1	F	201	ASN
1	F	206	GLU
1	F	212	LEU
1	F	333	THR
1	F	367	THR
1	G	2	LYS
1	G	51	THR
1	G	138	SER
1	G	201	ASN
1	G	206	GLU
1	G	244	LEU
1	G	306	SER
1	G	319	ARG
1	G	333	THR
1	G	362	ARG
1	H	51	THR
1	H	153	ARG
1	H	201	ASN
1	H	206	GLU
1	H	212	LEU
1	H	221	ILE
1	H	244	LEU
1	H	332	THR
1	H	333	THR
1	H	344	ARG

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Mol	Chain	Res	Type
1	H	353	ASP
1	H	367	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	B	9	HIS
1	B	29	HIS
1	B	201	ASN
1	C	201	ASN
1	D	9	HIS
1	D	83	GLN
1	D	84	HIS
1	D	157	GLN
1	D	201	ASN
1	E	83	GLN
1	E	157	GLN
1	E	201	ASN
1	E	320	HIS
1	F	29	HIS
1	F	83	GLN
1	F	201	ASN
1	G	29	HIS
1	G	201	ASN
1	H	83	GLN
1	H	201	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

8 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	PO4	A	401	-	4,4,4	0.55	0	6,6,6	0.35	0
2	PO4	B	401	-	4,4,4	0.33	0	6,6,6	0.29	0
2	PO4	C	401	-	4,4,4	0.20	0	6,6,6	0.32	0
2	PO4	D	401	-	4,4,4	0.77	0	6,6,6	0.34	0
2	PO4	E	401	-	4,4,4	0.65	0	6,6,6	0.34	0
2	PO4	F	401	-	4,4,4	0.45	0	6,6,6	0.32	0
2	PO4	G	401	-	4,4,4	0.58	0	6,6,6	0.29	0
2	PO4	H	401	-	4,4,4	0.64	0	6,6,6	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	401	-	-	0/0/0/0	0/0/0/0
2	PO4	B	401	-	-	0/0/0/0	0/0/0/0
2	PO4	C	401	-	-	0/0/0/0	0/0/0/0
2	PO4	D	401	-	-	0/0/0/0	0/0/0/0
2	PO4	E	401	-	-	0/0/0/0	0/0/0/0
2	PO4	F	401	-	-	0/0/0/0	0/0/0/0
2	PO4	G	401	-	-	0/0/0/0	0/0/0/0
2	PO4	H	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 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	372/386 (96%)	0.14	7 (1%) 70 70	19, 30, 42, 61	0
1	B	371/386 (96%)	0.62	38 (10%) 9 9	23, 35, 56, 73	0
1	C	372/386 (96%)	0.42	20 (5%) 29 31	23, 39, 53, 65	0
1	D	372/386 (96%)	0.23	11 (2%) 54 55	21, 31, 50, 57	0
1	E	372/386 (96%)	0.34	16 (4%) 39 40	21, 32, 45, 53	0
1	F	370/386 (95%)	0.56	41 (11%) 7 8	22, 34, 51, 60	0
1	G	372/386 (96%)	0.36	9 (2%) 62 63	22, 35, 53, 59	0
1	H	372/386 (96%)	0.40	19 (5%) 32 33	20, 34, 52, 61	0
All	All	2973/3088 (96%)	0.38	161 (5%) 29 31	19, 34, 51, 73	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	LEU	6.3
1	C	363	ASP	5.8
1	F	187	ALA	5.8
1	D	156	ALA	5.8
1	C	41	ASP	5.6
1	C	184	ALA	5.2
1	F	151	VAL	5.1
1	B	145	GLU	5.0
1	F	344	ARG	4.9
1	B	27	GLU	4.8
1	B	152	ALA	4.8
1	D	145	GLU	4.7
1	H	153	ARG	4.6
1	B	187	ALA	4.6
1	E	187	ALA	4.6
1	F	345	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	363	ASP	4.4
1	B	43	GLY	4.4
1	H	361	ASN	4.3
1	B	19	VAL	4.3
1	E	149	ALA	4.2
1	H	156	ALA	4.1
1	B	149	ALA	4.1
1	B	189	ARG	4.1
1	F	145	GLU	4.0
1	B	183	THR	4.0
1	A	361	ASN	3.9
1	E	184	ALA	3.9
1	F	139	ILE	3.9
1	C	153	ARG	3.8
1	H	363	ASP	3.8
1	B	28	TYR	3.6
1	B	156	ALA	3.6
1	F	149	ALA	3.6
1	F	190	GLN	3.6
1	B	23	SER	3.6
1	F	230[A]	TRP	3.5
1	A	145	GLU	3.4
1	G	367	THR	3.4
1	F	152	ALA	3.4
1	B	151	VAL	3.4
1	B	160	LYS	3.3
1	B	155	ARG	3.3
1	H	343	LEU	3.3
1	B	20	TYR	3.3
1	C	187	ALA	3.3
1	F	219	LEU	3.3
1	D	153	ARG	3.3
1	E	158	GLY	3.2
1	F	19	VAL	3.2
1	B	41	ASP	3.2
1	F	189	ARG	3.2
1	H	366	GLY	3.1
1	H	158	GLY	3.1
1	E	18	GLY	3.1
1	C	145	GLU	3.0
1	B	191	PRO	3.0
1	H	345	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	171	ALA	3.0
1	E	260	ILE	3.0
1	F	160	LYS	2.9
1	F	148	ARG	2.9
1	H	344	ARG	2.9
1	H	230[A]	TRP	2.9
1	B	186	LEU	2.8
1	B	231	ALA	2.8
1	B	17	GLY	2.8
1	F	186	LEU	2.8
1	F	147	MET	2.8
1	G	230[A]	TRP	2.8
1	A	230[A]	TRP	2.8
1	F	188	ASP	2.8
1	B	363	ASP	2.7
1	H	346	GLY	2.7
1	F	347	GLY	2.7
1	D	152	ALA	2.7
1	F	138	SER	2.7
1	F	28	TYR	2.7
1	F	156	ALA	2.7
1	F	159	PHE	2.7
1	C	345	ASP	2.7
1	C	359	ARG	2.7
1	F	22	LEU	2.7
1	B	159	PHE	2.7
1	F	137	SER	2.7
1	B	188	ASP	2.6
1	G	359	ARG	2.6
1	B	18	GLY	2.6
1	H	338	GLU	2.6
1	F	23	SER	2.6
1	F	21	ARG	2.6
1	A	365	LEU	2.6
1	A	364	ALA	2.6
1	F	146	ALA	2.5
1	F	180	GLU	2.5
1	B	148	ARG	2.5
1	E	192	GLY	2.5
1	C	361	ASN	2.5
1	E	191	PRO	2.5
1	B	42	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	151	VAL	2.5
1	F	353	ASP	2.5
1	E	146	ALA	2.5
1	G	1	LEU	2.5
1	B	29	HIS	2.5
1	H	367	THR	2.5
1	F	183	THR	2.4
1	H	151	VAL	2.4
1	C	144	PRO	2.4
1	C	338	GLU	2.4
1	E	345	ASP	2.4
1	C	230[A]	TRP	2.4
1	B	158	GLY	2.3
1	F	346	GLY	2.3
1	C	358	LEU	2.3
1	B	118	GLY	2.3
1	B	219	LEU	2.3
1	D	345	ASP	2.3
1	B	142	ASP	2.3
1	E	367	THR	2.3
1	D	149	ALA	2.3
1	E	119	LEU	2.3
1	A	359	ARG	2.2
1	F	287	ILE	2.2
1	B	230[A]	TRP	2.2
1	B	190	GLN	2.2
1	F	191	PRO	2.2
1	C	158	GLY	2.2
1	B	289	ALA	2.2
1	F	27	GLU	2.2
1	F	118	GLY	2.2
1	F	218	GLY	2.2
1	C	364	ALA	2.2
1	D	144	PRO	2.2
1	E	219	LEU	2.1
1	B	287	ILE	2.1
1	F	83	GLN	2.1
1	H	359	ARG	2.1
1	B	39	GLU	2.1
1	C	146	ALA	2.1
1	G	338	GLU	2.1
1	H	149	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	151	VAL	2.1
1	G	3	ILE	2.1
1	E	215	LEU	2.1
1	G	256	LEU	2.1
1	C	93	ASP	2.1
1	G	340	ASP	2.1
1	C	185	CYS	2.1
1	D	141	GLY	2.1
1	H	190	GLN	2.1
1	C	45	THR	2.1
1	D	187	ALA	2.0
1	E	188	ASP	2.0
1	E	19	VAL	2.0
1	F	20	TYR	2.0
1	F	153	ARG	2.0
1	D	157	GLN	2.0
1	H	340	ASP	2.0
1	G	353	ASP	2.0
1	H	339	ILE	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 carbohydrates 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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	A	401	5/5	0.96	0.16	2.43	35,36,40,44	0
2	PO4	F	401	5/5	0.95	0.16	2.18	34,36,36,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	B	401	5/5	0.95	0.16	1.62	38,42,45,48	0
2	PO4	E	401	5/5	0.97	0.16	0.72	41,43,44,46	0
2	PO4	H	401	5/5	0.98	0.14	0.08	38,39,39,43	0
2	PO4	G	401	5/5	0.97	0.15	-0.05	44,44,45,48	0
2	PO4	D	401	5/5	0.95	0.13	-1.01	31,34,39,43	0
2	PO4	C	401	5/5	0.97	0.09	-1.53	40,41,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.