Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2016 – 05:26 PM EDT

PDB ID	:	5HMQ
Title	:	xylose isomerase-like TIM barrel/4-hydroxyphenylpyruvate dioxygenase fusion protein
Authors	:	Peek, J.; Christendat, D.
Deposited on	:	2016-01-16
Resolution	:	2.37 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

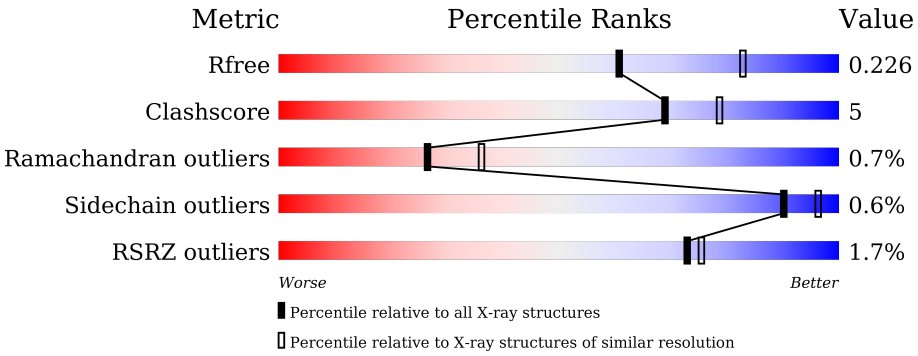
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.37 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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 <=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	637	2% 84% 13% ·
1	B	637	2% 90% 8% ·
1	C	637	% 86% 11% ·
1	D	637	2% 87% 10% ··
1	E	637	% 85% 12% ·
1	F	637	% 87% 10% ··

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	MG	A	701	-	-	-	X
2	MG	B	702	-	-	-	X
2	MG	E	701	-	-	-	X
2	MG	F	702	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30198 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 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	Se	0	0	0
			4850	3080	853	900	8	9			
1	B	621	Total	C	N	O	S	Se	0	0	0
			4854	3083	853	901	8	9			
1	C	622	Total	C	N	O	S	Se	0	0	0
			4824	3058	848	901	8	9			
1	D	624	Total	C	N	O	S	Se	0	0	0
			4869	3094	855	903	8	9			
1	E	621	Total	C	N	O	S	Se	0	0	0
			4845	3075	852	901	8	9			
1	F	623	Total	C	N	O	S	Se	0	0	0
			4860	3087	849	907	8	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP Q88JU3
A	0	LYS	-	expression tag	UNP Q88JU3
B	-1	ALA	-	expression tag	UNP Q88JU3
B	0	LYS	-	expression tag	UNP Q88JU3
C	-1	ALA	-	expression tag	UNP Q88JU3
C	0	LYS	-	expression tag	UNP Q88JU3
D	-1	ALA	-	expression tag	UNP Q88JU3
D	0	LYS	-	expression tag	UNP Q88JU3
E	-1	ALA	-	expression tag	UNP Q88JU3
E	0	LYS	-	expression tag	UNP Q88JU3
F	-1	ALA	-	expression tag	UNP Q88JU3
F	0	LYS	-	expression tag	UNP Q88JU3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0

- Molecule 3 is water.

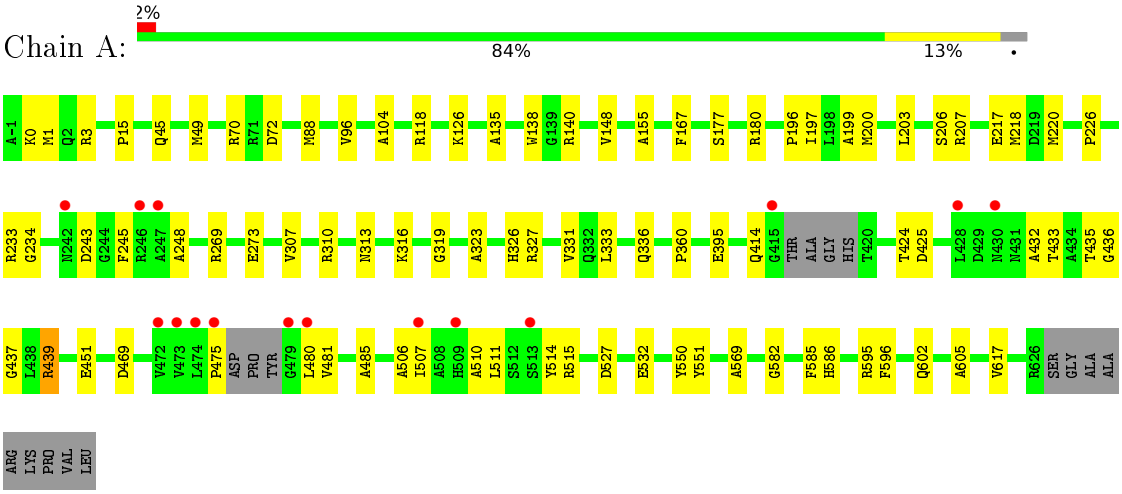
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	140	Total O 140 140	0	0
3	B	195	Total O 195 195	0	0
3	C	128	Total O 128 128	0	0
3	D	231	Total O 231 231	0	0
3	E	236	Total O 236 236	0	0
3	F	154	Total O 154 154	0	0

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.

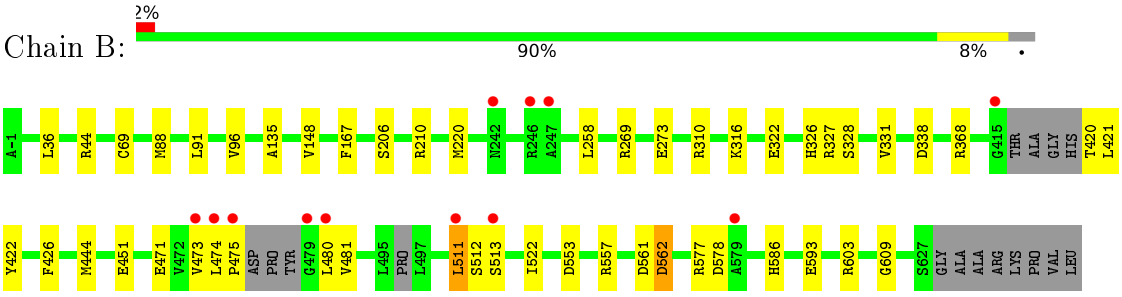
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

Chain A:



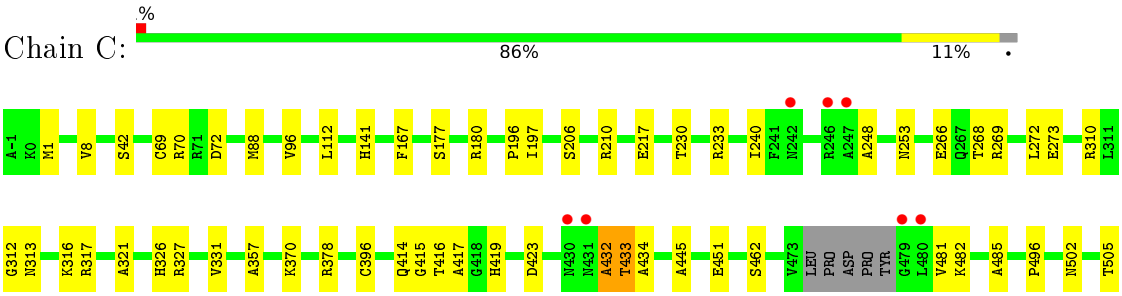
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

Chain B:

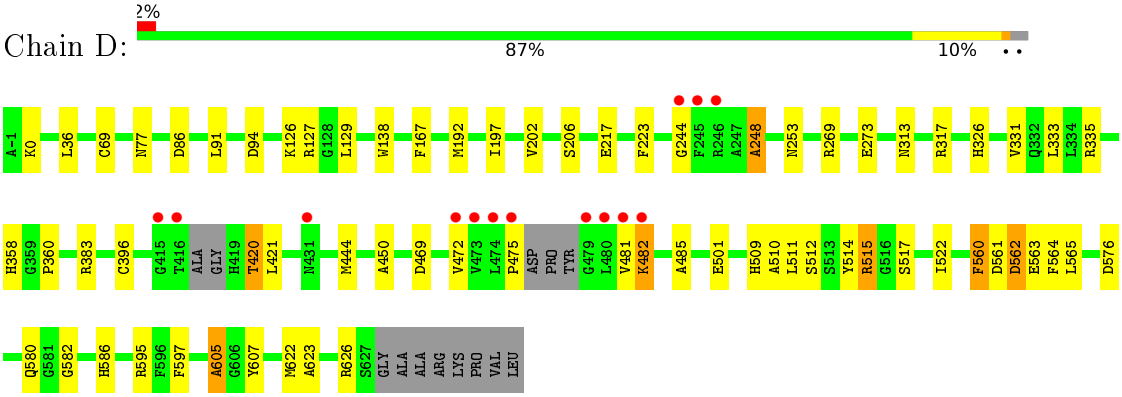


- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

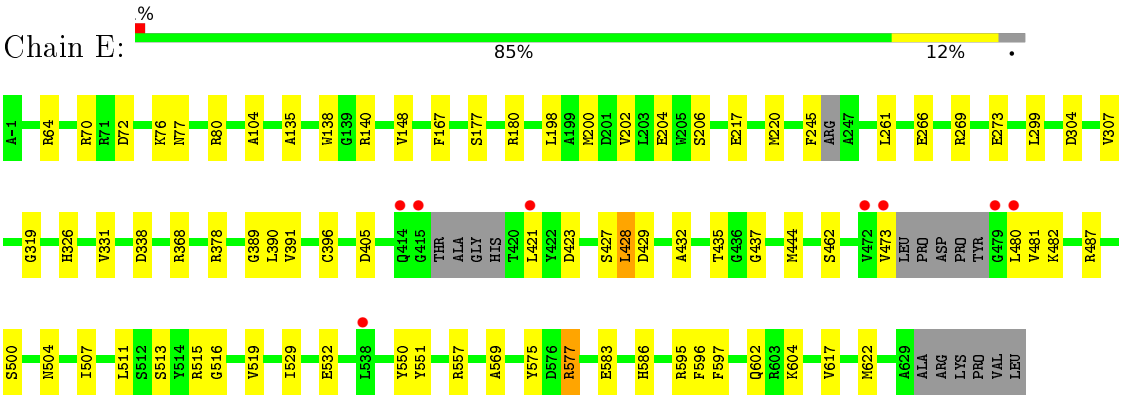
Chain C:



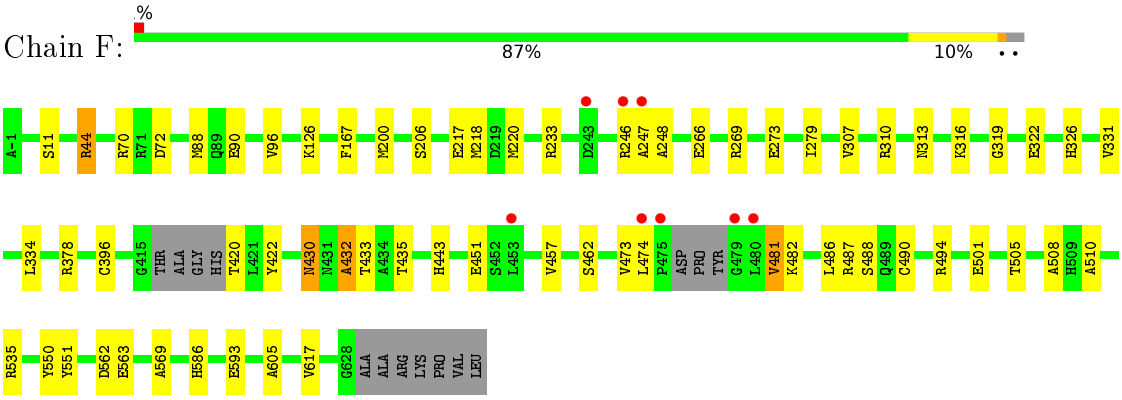
• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	262.50Å 262.50Å 139.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.44 – 2.37 88.15 – 2.37	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.44-2.37) 95.6 (88.15-2.37)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.204 , 0.229 0.200 , 0.226	Depositor DCC
R_{free} test set	10631 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 19.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.126 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	30198	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.29	0/4946	0.51	2/6682 (0.0%)
1	B	0.30	0/4948	0.50	1/6684 (0.0%)
1	C	0.29	0/4918	0.49	1/6645 (0.0%)
1	D	0.30	0/4966	0.54	4/6713 (0.1%)
1	E	0.30	0/4939	0.51	3/6672 (0.0%)
1	F	0.29	0/4956	0.50	1/6699 (0.0%)
All	All	0.30	0/29673	0.51	12/40095 (0.0%)

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	511	LEU	CB-CG-CD1	-10.27	93.54	111.00
1	B	511	LEU	CB-CG-CD2	8.96	126.22	111.00
1	D	515	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	D	472	VAL	CG1-CB-CG2	-6.82	99.99	110.90
1	F	481	VAL	CG1-CB-CG2	6.23	120.87	110.90
1	E	511	LEU	CB-CG-CD2	-6.21	100.44	111.00
1	E	473	VAL	CG1-CB-CG2	6.14	120.73	110.90
1	A	439	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	A	439	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	C	511	LEU	CA-CB-CG	5.53	128.01	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	126	LYS	CB-CG-CD	-5.36	97.67	111.60
1	E	513	SER	N-CA-CB	5.24	118.36	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	471	GLU	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	4850	0	4743	54	0
1	B	4854	0	4750	32	0
1	C	4824	0	4697	53	0
1	D	4869	0	4759	50	0
1	E	4845	0	4729	56	0
1	F	4860	0	4745	43	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	140	0	0	2	0
3	B	195	0	0	4	0
3	C	128	0	0	3	0
3	D	231	0	0	5	0
3	E	236	0	0	5	0
3	F	154	0	0	2	0
All	All	30198	0	28423	265	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 (265) 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:217:GLU:OE1	1:E:482:LYS:NZ	1.94	0.99
1:E:427:SER:HA	1:E:428:LEU:HB2	1.42	0.99
1:C:502:ASN:OD1	1:C:505:THR:N	2.05	0.89
1:B:511:LEU:HD23	1:B:513:SER:H	1.37	0.89
1:B:603:ARG:NH2	1:B:609:GLY:O	2.07	0.87
1:A:439:ARG:HH12	1:A:527:ASP:CG	1.79	0.85
1:D:444:MSE:HE2	1:D:522:ILE:HG12	1.60	0.84
1:E:104:ALA:O	1:E:140:ARG:NH1	2.14	0.81
1:C:327:ARG:NH2	1:C:423:ASP:O	2.16	0.79
1:D:482:LYS:HZ3	1:E:507:ILE:HG22	1.46	0.79
1:E:396:CYS:SG	3:E:1012:HOH:O	2.41	0.78
1:D:482:LYS:NZ	1:E:507:ILE:HG22	1.98	0.78
1:D:515:ARG:HA	1:D:515:ARG:NE	2.00	0.77
1:D:515:ARG:NH2	1:E:204:GLU:OE1	2.18	0.76
1:F:396:CYS:SG	3:F:944:HOH:O	2.43	0.75
1:E:64:ARG:O	1:E:80:ARG:NH2	2.19	0.75
1:B:338:ASP:OD2	1:B:368:ARG:NH2	2.18	0.75
1:D:129:LEU:HB3	3:D:801:HOH:O	1.87	0.74
1:C:70:ARG:NH2	1:C:72:ASP:OD2	2.20	0.74
1:D:562:ASP:O	1:D:564:PHE:N	2.19	0.73
1:A:507:ILE:HG22	1:C:482:LYS:NZ	2.03	0.73
1:B:553:ASP:OD1	1:B:557:ARG:NH1	2.22	0.73
1:D:396:CYS:SG	3:D:997:HOH:O	2.46	0.72
1:C:197:ILE:HG12	1:C:217:GLU:HG3	1.72	0.72
1:F:247:ALA:H	1:F:248:ALA:HB2	1.55	0.71
1:C:396:CYS:SG	3:C:923:HOH:O	2.49	0.71
1:A:582:GLY:HA2	1:A:605:ALA:HB3	1.72	0.69
1:B:473:VAL:HG12	1:B:474:LEU:H	1.59	0.67
1:E:583:GLU:OE1	1:E:604:LYS:NZ	2.26	0.67
1:E:70:ARG:NH1	1:E:72:ASP:OD1	2.27	0.67
1:B:69:CYS:SG	3:B:978:HOH:O	2.52	0.66
1:B:327:ARG:NH1	1:B:426:PHE:O	2.28	0.66
1:B:473:VAL:HG12	1:B:474:LEU:HD12	1.77	0.66
1:F:473:VAL:HG22	1:F:474:LEU:H	1.60	0.66
1:C:69:CYS:SG	3:C:925:HOH:O	2.53	0.65
1:C:506:ALA:HA	1:C:511:LEU:HD13	1.76	0.65
1:C:326:HIS:HB2	1:C:331:VAL:HB	1.79	0.65
1:D:515:ARG:HA	1:D:515:ARG:HE	1.62	0.64
1:C:603:ARG:NH2	1:C:609:GLY:O	2.31	0.64
1:A:414:GLN:NE2	3:A:803:HOH:O	2.30	0.64
1:B:475:PRO:HA	1:B:481:VAL:HG12	1.80	0.64
1:E:266:GLU:OE2	1:E:378:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:217:GLU:OE2	1:F:482:LYS:NZ	2.24	0.64
1:A:15:PRO:HB3	1:A:49:MSE:HE1	1.79	0.63
1:D:192:MSE:HE1	1:D:223:PHE:HD2	1.64	0.63
1:B:420:THR:O	1:B:422:TYR:N	2.31	0.63
1:D:383:ARG:NH2	3:D:802:HOH:O	2.32	0.63
1:D:86:ASP:OD1	1:D:127:ARG:NH2	2.26	0.62
1:D:333:LEU:HD21	1:D:335:ARG:HH21	1.64	0.62
1:E:557:ARG:NH2	3:E:805:HOH:O	2.33	0.62
1:D:580:GLN:O	1:D:580:GLN:HG2	2.00	0.62
1:C:1:MSE:HE3	1:C:233:ARG:HA	1.82	0.62
1:D:420:THR:OG1	1:D:421:LEU:N	2.31	0.61
1:E:427:SER:CA	1:E:428:LEU:HB2	2.26	0.61
1:E:389:GLY:HA3	1:E:391:VAL:HG23	1.82	0.61
1:F:473:VAL:HG12	1:F:481:VAL:O	2.01	0.61
1:A:514:TYR:O	1:A:515:ARG:NH1	2.30	0.60
1:A:327:ARG:NE	1:A:424:THR:O	2.34	0.60
1:E:529:ILE:N	1:E:602:GLN:OE1	2.30	0.60
1:F:44:ARG:NE	1:F:90:GLU:OE1	2.35	0.60
1:F:247:ALA:HB3	1:F:248:ALA:HA	1.83	0.59
1:D:358:HIS:O	1:D:595:ARG:NH2	2.33	0.59
1:B:511:LEU:HD23	1:B:513:SER:N	2.12	0.59
1:C:370:LYS:HA	1:C:414:GLN:HE22	1.68	0.58
1:A:507:ILE:HG22	1:C:482:LYS:HZ1	1.68	0.58
1:E:140:ARG:NH1	3:E:806:HOH:O	2.36	0.58
1:E:575:TYR:OH	1:E:577:ARG:NE	2.26	0.58
1:C:310:ARG:NH1	1:C:593:GLU:OE2	2.28	0.57
1:D:94:ASP:O	3:D:801:HOH:O	2.18	0.57
1:A:88:MSE:SE	1:A:96:VAL:HB	2.54	0.57
1:C:378:ARG:NH1	1:C:462:SER:O	2.38	0.57
1:C:414:GLN:CD	1:C:414:GLN:H	2.07	0.57
1:F:432:ALA:CB	1:F:433:THR:HA	2.35	0.57
1:D:482:LYS:NZ	1:E:507:ILE:CG2	2.68	0.56
1:E:76:LYS:NZ	3:E:801:HOH:O	2.22	0.56
1:F:562:ASP:OD2	1:F:563:GLU:OE2	2.23	0.56
1:A:126:LYS:HE3	1:F:126:LYS:HD2	1.86	0.56
1:B:557:ARG:NH2	3:B:804:HOH:O	2.37	0.56
1:F:167:PHE:CE1	1:F:206:SER:HB2	2.41	0.55
1:D:383:ARG:NH1	3:D:806:HOH:O	2.39	0.55
1:C:370:LYS:HA	1:C:414:GLN:NE2	2.21	0.55
1:F:378:ARG:NH1	1:F:462:SER:O	2.40	0.55
1:C:196:PRO:HA	1:C:217:GLU:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ARG:NH2	3:B:805:HOH:O	2.40	0.55
1:E:198:LEU:HD13	1:E:200:MSE:HE3	1.89	0.55
1:A:550:TYR:CD1	1:A:617:VAL:HG21	2.42	0.54
1:A:439:ARG:NH1	1:A:527:ASP:OD2	2.36	0.54
1:D:326:HIS:HB2	1:D:331:VAL:HB	1.90	0.54
1:E:427:SER:HA	1:E:428:LEU:CB	2.27	0.54
1:F:70:ARG:NH2	1:F:72:ASP:OD2	2.25	0.54
1:E:177:SER:O	1:E:180:ARG:HG2	2.07	0.54
1:A:200:MSE:HE2	1:C:512:SER:HA	1.90	0.54
1:D:475:PRO:HD3	1:D:481:VAL:HG12	1.90	0.54
1:D:360:PRO:HD2	1:D:595:ARG:NH1	2.22	0.54
1:A:327:ARG:HG3	1:A:425:ASP:O	2.08	0.54
1:C:177:SER:O	1:C:180:ARG:HG2	2.08	0.54
1:C:268:THR:O	1:C:272:LEU:HD22	2.08	0.54
1:C:266:GLU:OE2	1:C:378:ARG:NH2	2.41	0.53
1:B:269:ARG:O	1:B:273:GLU:HG3	2.09	0.53
1:E:421:LEU:H	1:E:421:LEU:HD23	1.74	0.52
1:D:482:LYS:HZ1	1:E:507:ILE:CG2	2.22	0.52
1:F:490:CYS:SG	3:F:943:HOH:O	2.59	0.52
1:A:336:GLN:OE1	1:A:436:GLY:HA3	2.10	0.52
1:C:419:HIS:O	1:C:423:ASP:HB2	2.10	0.51
1:A:167:PHE:CE1	1:A:206:SER:HB2	2.45	0.51
1:A:326:HIS:HB2	1:A:331:VAL:HB	1.92	0.51
1:C:141:HIS:ND1	3:C:802:HOH:O	2.34	0.51
1:D:167:PHE:CE1	1:D:206:SER:HB2	2.45	0.51
1:D:512:SER:HA	1:E:200:MSE:HE2	1.93	0.51
1:A:395:GLU:OE2	3:A:801:HOH:O	2.19	0.51
1:B:316:LYS:NZ	1:B:322:GLU:OE2	2.30	0.51
1:E:167:PHE:CE1	1:E:206:SER:HB2	2.46	0.51
1:A:269:ARG:O	1:A:273:GLU:HG3	2.10	0.51
1:C:312:GLY:O	1:C:316:LYS:HG2	2.10	0.51
1:E:423:ASP:OD1	1:E:428:LEU:HD21	2.11	0.51
1:F:550:TYR:CD1	1:F:617:VAL:HG21	2.46	0.51
1:A:1:MSE:HE3	1:A:233:ARG:HA	1.93	0.50
1:E:378:ARG:NH1	1:E:462:SER:O	2.44	0.50
1:E:319:GLY:HA2	1:E:435:THR:OG1	2.11	0.50
1:E:338:ASP:OD1	1:E:368:ARG:NH2	2.43	0.50
1:A:507:ILE:HG22	1:C:482:LYS:HZ2	1.75	0.50
1:A:45:GLN:O	1:A:49:MSE:HG3	2.12	0.49
1:B:451:GLU:H	1:B:451:GLU:CD	2.15	0.49
1:D:515:ARG:CA	1:D:515:ARG:NE	2.69	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:551:TYR:CZ	1:E:569:ALA:HA	2.47	0.49
1:F:551:TYR:CZ	1:F:569:ALA:HA	2.48	0.49
1:C:269:ARG:O	1:C:273:GLU:HG3	2.13	0.49
1:B:167:PHE:CE1	1:B:206:SER:HB2	2.48	0.48
1:C:445:ALA:HB2	1:C:496:PRO:HG2	1.95	0.48
1:F:435:THR:O	1:F:535:ARG:HD2	2.14	0.48
1:C:167:PHE:CE1	1:C:206:SER:HB2	2.49	0.48
1:D:36:LEU:HD11	1:D:91:LEU:HD11	1.95	0.48
1:A:313:ASN:HA	1:A:316:LYS:HE3	1.96	0.48
1:C:180:ARG:HA	1:C:230:THR:HG22	1.94	0.48
1:E:77:ASN:OD1	1:E:80:ARG:NH1	2.47	0.48
1:A:207:ARG:HD2	1:C:357:ALA:O	2.14	0.47
1:D:450:ALA:O	1:E:504:ASN:ND2	2.48	0.47
1:E:326:HIS:HB2	1:E:331:VAL:HB	1.96	0.47
1:E:597:PHE:CG	1:E:622:MSE:HE1	2.49	0.47
1:F:501:GLU:OE2	1:F:505:THR:HG21	2.14	0.47
1:F:269:ARG:O	1:F:273:GLU:HG3	2.14	0.47
1:D:269:ARG:O	1:D:273:GLU:HG3	2.15	0.47
1:A:197:ILE:HD12	1:A:217:GLU:HB2	1.97	0.47
1:F:481:VAL:HG23	1:F:482:LYS:N	2.30	0.47
1:A:199:ALA:O	1:C:512:SER:HB2	2.15	0.47
1:A:506:ALA:HA	1:A:511:LEU:HD12	1.96	0.46
1:A:510:ALA:HB2	1:C:481:VAL:HG21	1.97	0.46
1:B:36:LEU:HD11	1:B:91:LEU:HD11	1.96	0.46
1:C:567:GLU:O	1:C:571:TYR:HD1	1.99	0.46
1:E:515:ARG:HD2	1:E:595:ARG:HE	1.81	0.46
1:A:307:VAL:HG11	1:A:360:PRO:HG3	1.97	0.46
1:B:473:VAL:HG23	1:B:481:VAL:O	2.16	0.46
1:C:509:HIS:HB2	1:C:511:LEU:CD1	2.45	0.46
1:E:519:VAL:HG13	1:E:596:PHE:HB3	1.98	0.46
1:C:210:ARG:HB3	1:C:240:ILE:HD12	1.97	0.46
1:F:88:MSE:SE	1:F:96:VAL:HB	2.65	0.46
1:A:138:TRP:CE2	1:A:203:LEU:HD12	2.51	0.46
1:A:118:ARG:HD3	1:A:155:ALA:O	2.15	0.46
1:C:485:ALA:HA	1:C:496:PRO:HA	1.98	0.46
1:F:322:GLU:HG2	1:F:334:LEU:HD21	1.96	0.46
1:E:550:TYR:CD1	1:E:617:VAL:HG21	2.51	0.46
1:A:319:GLY:HA2	1:A:435:THR:OG1	2.16	0.46
1:F:307:VAL:HG22	1:F:310:ARG:NH2	2.30	0.46
1:B:481:VAL:HG21	1:F:510:ALA:HB2	1.97	0.46
1:A:307:VAL:HG22	1:A:310:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:LYS:HD2	1:A:3:ARG:NH1	2.31	0.45
1:A:218:MSE:HB2	1:A:220:MSE:HE3	1.97	0.45
1:E:138:TRP:HE3	1:E:202:VAL:HG13	1.82	0.45
1:C:509:HIS:HB2	1:C:511:LEU:HD12	1.98	0.45
1:E:299:LEU:HD22	1:E:444:MSE:HE1	1.98	0.45
1:F:443:HIS:HB3	1:F:494:ARG:HB2	1.99	0.45
1:B:310:ARG:NH1	1:B:593:GLU:OE1	2.50	0.45
1:D:248:ALA:HB1	1:D:253:ASN:ND2	2.31	0.45
1:C:451:GLU:H	1:C:451:GLU:CD	2.19	0.45
1:F:233:ARG:NH2	1:F:279:ILE:HD11	2.32	0.45
1:E:269:ARG:O	1:E:273:GLU:HG3	2.16	0.45
1:C:313:ASN:HB3	1:C:317:ARG:NH1	2.31	0.45
1:C:505:THR:HG23	1:C:509:HIS:CD2	2.52	0.45
1:A:551:TYR:CZ	1:A:569:ALA:HA	2.52	0.44
1:D:197:ILE:HD12	1:D:217:GLU:HB2	2.00	0.44
1:E:480:LEU:HD23	1:E:481:VAL:N	2.33	0.44
1:D:444:MSE:CE	1:D:522:ILE:HG12	2.40	0.44
1:E:429:ASP:CG	1:E:432:ALA:HB2	2.37	0.44
1:C:543:LEU:HD23	1:C:589:THR:HG22	1.99	0.44
1:B:444:MSE:SE	1:B:522:ILE:HG12	2.68	0.44
1:B:577:ARG:HG2	1:B:578:ASP:O	2.18	0.44
1:D:244:GLY:O	1:E:405:ASP:HA	2.17	0.44
1:D:248:ALA:HB1	1:D:253:ASN:HD21	1.81	0.44
1:E:389:GLY:HA3	1:E:390:LEU:C	2.38	0.44
1:F:266:GLU:OE2	1:F:378:ARG:NH2	2.51	0.44
1:D:626:ARG:HA	1:D:626:ARG:HD3	1.84	0.44
1:C:88:MSE:SE	1:C:96:VAL:HB	2.68	0.44
1:A:469:ASP:O	1:A:485:ALA:HB3	2.17	0.43
1:C:414:GLN:CD	1:C:414:GLN:N	2.71	0.43
1:F:11:SER:OG	1:F:248:ALA:HB3	2.18	0.43
1:B:480:LEU:HG	1:F:508:ALA:HB1	2.00	0.43
1:A:70:ARG:NE	1:A:72:ASP:OD1	2.51	0.43
1:A:595:ARG:HB2	1:A:596:PHE:H	1.47	0.43
1:C:316:LYS:H	1:C:316:LYS:HG2	1.63	0.43
1:F:451:GLU:H	1:F:451:GLU:CD	2.22	0.43
1:B:135:ALA:HB2	1:B:148:VAL:HG23	2.00	0.43
1:C:248:ALA:HB1	1:C:253:ASN:HD21	1.83	0.43
1:D:597:PHE:CG	1:D:622:MSE:HE1	2.54	0.43
1:B:512:SER:HA	1:F:200:MSE:HE2	2.00	0.43
1:A:451:GLU:CD	1:A:451:GLU:H	2.22	0.43
1:A:480:LEU:H	1:A:480:LEU:HD12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:O	1:A:180:ARG:HG3	2.19	0.42
1:A:180:ARG:HG3	1:A:226:PRO:HB3	2.01	0.42
1:F:473:VAL:HG22	1:F:474:LEU:N	2.31	0.42
1:D:623:ALA:O	1:D:626:ARG:HG2	2.19	0.42
1:E:220:MSE:HA	1:E:220:MSE:HE2	2.02	0.42
1:F:313:ASN:HA	1:F:316:LYS:HE3	2.02	0.42
1:A:439:ARG:NH1	1:A:527:ASP:CG	2.59	0.42
1:A:245:PHE:CD2	1:C:517:SER:HB2	2.55	0.42
1:A:196:PRO:HG3	1:C:507:ILE:HD13	2.01	0.42
1:D:138:TRP:HE3	1:D:202:VAL:HG13	1.85	0.42
1:E:261:LEU:HA	1:E:261:LEU:HD23	1.93	0.42
1:A:323:ALA:HB3	1:A:333:LEU:HG	2.01	0.42
1:D:192:MSE:HE1	1:D:223:PHE:CD2	2.50	0.42
1:E:480:LEU:HD21	1:E:482:LYS:O	2.20	0.42
1:F:220:MSE:HA	1:F:220:MSE:HE2	2.02	0.42
1:F:310:ARG:NE	1:F:593:GLU:OE2	2.45	0.42
1:D:623:ALA:O	1:D:626:ARG:N	2.48	0.41
1:B:474:LEU:HD12	1:B:474:LEU:H	1.86	0.41
1:C:595:ARG:HB2	1:C:596:PHE:H	1.56	0.41
1:D:313:ASN:O	1:D:317:ARG:HG3	2.19	0.41
1:B:511:LEU:CD2	1:B:513:SER:H	2.21	0.41
1:C:8:VAL:HG13	1:C:240:ILE:O	2.19	0.41
1:D:69:CYS:SG	1:D:77:ASN:ND2	2.92	0.41
1:D:469:ASP:O	1:D:485:ALA:HB3	2.20	0.41
1:E:304:ASP:OD1	1:E:307:VAL:HG12	2.21	0.41
1:F:218:MSE:HB2	1:F:220:MSE:HE3	2.02	0.41
1:F:326:HIS:HB2	1:F:331:VAL:HB	2.01	0.41
1:A:104:ALA:HA	1:A:140:ARG:HE	1.85	0.41
1:B:220:MSE:HE2	1:B:220:MSE:HA	2.02	0.41
1:B:326:HIS:HB2	1:B:331:VAL:HB	2.02	0.41
1:F:430:ASN:C	1:F:432:ALA:N	2.73	0.41
1:F:457:VAL:HA	1:F:486:LEU:HD11	2.02	0.41
1:C:502:ASN:C	1:C:502:ASN:OD1	2.59	0.41
1:A:135:ALA:HB2	1:A:148:VAL:HG23	2.03	0.41
1:D:501:GLU:O	1:D:514:TYR:HE1	2.04	0.41
1:D:576:ASP:OD2	1:D:607:TYR:OH	2.29	0.41
1:D:517:SER:HB2	1:E:245:PHE:CD2	2.56	0.41
1:A:475:PRO:HG3	1:A:481:VAL:HG22	2.03	0.41
1:B:88:MSE:SE	1:B:96:VAL:HB	2.71	0.41
1:E:437:GLY:H	1:E:532:GLU:CD	2.24	0.41
1:E:575:TYR:OH	1:E:583:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:ALA:HB2	1:E:148:VAL:HG23	2.03	0.41
1:F:420:THR:O	1:F:422:TYR:N	2.53	0.41
1:F:451:GLU:N	1:F:451:GLU:OE1	2.49	0.41
1:A:515:ARG:HA	1:A:515:ARG:HD3	1.81	0.41
1:D:582:GLY:HA2	1:D:605:ALA:HB3	2.01	0.41
1:F:487:ARG:HG2	1:F:488:SER:O	2.21	0.41
1:B:210:ARG:HB2	3:B:935:HOH:O	2.21	0.40
1:C:432:ALA:O	1:C:433:THR:OG1	2.39	0.40
1:D:560:PHE:CD2	1:D:565:LEU:HD12	2.55	0.40
1:F:319:GLY:HA2	1:F:435:THR:OG1	2.20	0.40
1:D:244:GLY:HA3	1:E:405:ASP:O	2.21	0.40
1:D:515:ARG:HH12	1:D:595:ARG:NH1	2.18	0.40
1:E:487:ARG:HB3	1:E:487:ARG:CZ	2.51	0.40
1:A:1:MSE:HE2	1:A:234:GLY:O	2.21	0.40
1:A:437:GLY:HA2	1:A:532:GLU:OE2	2.20	0.40
1:A:585:PHE:O	1:A:602:GLN:N	2.50	0.40
1:E:519:VAL:HG12	3:E:974:HOH:O	2.20	0.40
1:C:321:ALA:HB2	1:C:434:ALA:HA	2.04	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	615/637 (96%)	592 (96%)	19 (3%)	4 (1%)	26	36
1	B	613/637 (96%)	597 (97%)	13 (2%)	3 (0%)	34	46
1	C	618/637 (97%)	593 (96%)	19 (3%)	6 (1%)	19	26
1	D	618/637 (97%)	593 (96%)	17 (3%)	8 (1%)	15	19
1	E	613/637 (96%)	601 (98%)	10 (2%)	2 (0%)	46	61
1	F	617/637 (97%)	597 (97%)	16 (3%)	4 (1%)	30	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3694/3822 (97%)	3573 (97%)	94 (2%)	27 (1%)	26 36

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	A	432	ALA
1	A	433	THR
1	B	562	ASP
1	C	433	THR
1	D	420	THR
1	D	605	ALA
1	E	428	LEU
1	F	430	ASN
1	F	432	ALA
1	F	605	ALA
1	B	421	LEU
1	B	561	ASP
1	C	417	ALA
1	C	432	ALA
1	D	563	GLU
1	F	246	ARG
1	C	516	GLY
1	D	560	PHE
1	E	516	GLY
1	C	415	GLY
1	C	416	THR
1	D	248	ALA
1	D	561	ASP
1	D	510	ALA
1	D	562	ASP
1	A	248	ALA

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	495/501 (99%)	494 (100%)	1 (0%)	95 99
1	B	496/501 (99%)	491 (99%)	5 (1%)	82 92
1	C	490/501 (98%)	487 (99%)	3 (1%)	90 96
1	D	497/501 (99%)	493 (99%)	4 (1%)	86 94
1	E	494/501 (99%)	491 (99%)	3 (1%)	90 96
1	F	497/501 (99%)	495 (100%)	2 (0%)	93 98
All	All	2969/3006 (99%)	2951 (99%)	18 (1%)	90 96

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	586	HIS
1	B	44	ARG
1	B	258	LEU
1	B	328	SER
1	B	562	ASP
1	B	586	HIS
1	C	42	SER
1	C	112	LEU
1	C	586	HIS
1	D	0	LYS
1	D	482	LYS
1	D	509	HIS
1	D	586	HIS
1	E	500	SER
1	E	577	ARG
1	E	586	HIS
1	F	44	ARG
1	F	586	HIS

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

Mol	Chain	Res	Type
1	C	373	GLN
1	E	373	GLN
1	F	580	GLN

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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	612/637 (96%)	0.01	15 (2%)	61	64	38, 51, 70, 90	0
1	B	612/637 (96%)	-0.09	12 (1%)	68	71	34, 44, 70, 96	0
1	C	613/637 (96%)	-0.08	7 (1%)	82	84	37, 50, 76, 98	0
1	D	615/637 (96%)	0.02	14 (2%)	64	67	31, 44, 75, 100	0
1	E	612/637 (96%)	0.01	8 (1%)	79	81	30, 44, 71, 83	0
1	F	614/637 (96%)	-0.10	8 (1%)	79	81	35, 47, 67, 96	0
All	All	3678/3822 (96%)	-0.04	64 (1%)	73	75	30, 47, 72, 100	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	GLY	9.7
1	B	475	PRO	9.1
1	B	480	LEU	7.2
1	B	474	LEU	6.8
1	D	480	LEU	6.8
1	D	474	LEU	6.2
1	A	480	LEU	6.1
1	A	474	LEU	6.0
1	F	479	GLY	5.8
1	A	473	VAL	5.4
1	F	480	LEU	5.3
1	E	415	GLY	5.1
1	A	475	PRO	5.1
1	A	247	ALA	5.1
1	E	473	VAL	5.1
1	B	246	ARG	5.1
1	C	479	GLY	5.1
1	E	480	LEU	4.8
1	D	473	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	247	ALA	4.5
1	B	247	ALA	4.4
1	B	479	GLY	4.3
1	C	480	LEU	4.3
1	A	509	HIS	4.1
1	D	472	VAL	4.1
1	D	475	PRO	3.8
1	B	473	VAL	3.7
1	E	472	VAL	3.6
1	E	414	GLN	3.5
1	D	479	GLY	3.2
1	A	507	ILE	3.1
1	C	246	ARG	3.1
1	E	479	GLY	3.0
1	B	513	SER	2.9
1	F	474	LEU	2.8
1	A	513	SER	2.8
1	A	246	ARG	2.8
1	D	416	THR	2.7
1	F	243	ASP	2.7
1	A	415	GLY	2.7
1	A	428	LEU	2.5
1	D	246	ARG	2.5
1	C	431	ASN	2.5
1	A	430	ASN	2.4
1	E	421	LEU	2.4
1	B	511	LEU	2.4
1	C	242	ASN	2.4
1	B	242	ASN	2.3
1	D	431	ASN	2.3
1	A	479	GLY	2.3
1	B	579	ALA	2.3
1	D	481	VAL	2.2
1	F	246	ARG	2.2
1	C	247	ALA	2.2
1	F	453	LEU	2.2
1	F	475	PRO	2.2
1	A	242	ASN	2.1
1	E	538	LEU	2.1
1	B	415	GLY	2.1
1	D	482	LYS	2.1
1	D	244	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	245	PHE	2.1
1	C	430	ASN	2.0
1	A	472	VAL	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	A	701	1/1	0.93	0.18	4.46	45,45,45,45	0
2	MG	E	701	1/1	0.98	0.16	3.38	30,30,30,30	0
2	MG	F	702	1/1	0.98	0.14	3.04	34,34,34,34	0
2	MG	B	702	1/1	0.98	0.16	2.10	38,38,38,38	0
2	MG	A	702	1/1	0.98	0.13	0.77	44,44,44,44	0
2	MG	C	702	1/1	0.93	0.13	0.76	45,45,45,45	0
2	MG	B	701	1/1	0.94	0.11	-0.81	38,38,38,38	0
2	MG	E	702	1/1	0.97	0.11	-0.88	42,42,42,42	0
2	MG	C	701	1/1	0.99	0.07	-2.10	43,43,43,43	0
2	MG	D	701	1/1	0.98	0.08	-2.71	33,33,33,33	0
2	MG	D	702	1/1	0.92	0.08	-4.15	47,47,47,47	0
2	MG	F	701	1/1	0.98	0.05	-9.29	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.