Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:10 PM GMT

PDB ID	:	3WB8
Title	:	Crystal Structure of MyoVa-GTD
Authors	:	Wei, Z.; Liu, X.; Yu, C.; Zhang, M.
Deposited on	:	2013-05-13
Resolution	:	2.50 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:

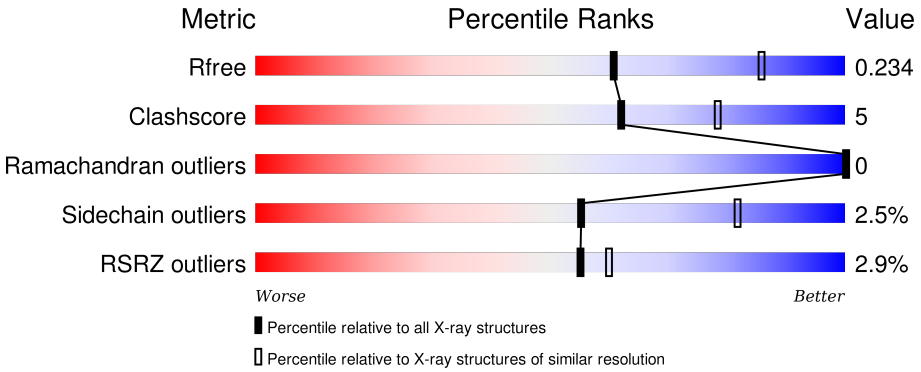
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	404	77% 12% 10%
1	B	404	4% 73% 13% 14%
1	C	404	74% 15% 11%
1	D	404	76% 12% • 11%
1	E	404	2% 77% 11% • 11%

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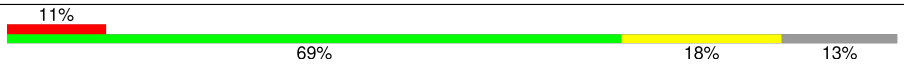
Mol	Chain	Length	Quality of chain
1	F	404	
1	G	404	
1	H	404	

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	EDO	A	1902	-	-	-	X
2	EDO	A	1904	-	-	-	X
2	EDO	B	1902	-	-	-	X
2	EDO	C	1902	-	-	-	X
2	EDO	D	1903	-	-	-	X
2	EDO	E	1902	-	-	-	X
2	EDO	G	1902	-	-	-	X
2	EDO	H	1902	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23277 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 Unconventional myosin-Va.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2913	1855	500	536	22			
1	B	348	Total	C	N	O	S	0	0	0
			2740	1747	465	507	21			
1	C	359	Total	C	N	O	S	0	1	0
			2890	1839	502	527	22			
1	D	360	Total	C	N	O	S	0	0	0
			2876	1826	496	532	22			
1	E	361	Total	C	N	O	S	0	0	0
			2883	1833	498	530	22			
1	F	359	Total	C	N	O	S	0	0	0
			2873	1830	495	526	22			
1	G	360	Total	C	N	O	S	0	0	0
			2907	1849	501	535	22			
1	H	352	Total	C	N	O	S	0	0	0
			2751	1747	469	514	21			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1450	HIS	-	EXPRESSION TAG	UNP Q99104
A	1451	HIS	-	EXPRESSION TAG	UNP Q99104
A	1452	HIS	-	EXPRESSION TAG	UNP Q99104
A	1453	HIS	-	EXPRESSION TAG	UNP Q99104
A	1454	HIS	-	EXPRESSION TAG	UNP Q99104
A	1455	HIS	-	EXPRESSION TAG	UNP Q99104
A	1456	SER	-	EXPRESSION TAG	UNP Q99104
A	1457	SER	-	EXPRESSION TAG	UNP Q99104
A	1458	GLY	-	EXPRESSION TAG	UNP Q99104
A	1459	LEU	-	EXPRESSION TAG	UNP Q99104
A	1460	GLY	-	EXPRESSION TAG	UNP Q99104
A	1461	VAL	-	EXPRESSION TAG	UNP Q99104
A	1462	LEU	-	EXPRESSION TAG	UNP Q99104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1463	PHE	-	EXPRESSION TAG	UNP Q99104
A	1464	GLN	-	EXPRESSION TAG	UNP Q99104
A	1465	GLY	-	EXPRESSION TAG	UNP Q99104
A	1466	PRO	-	EXPRESSION TAG	UNP Q99104
A	1467	GLY	-	EXPRESSION TAG	UNP Q99104
A	1468	SER	-	EXPRESSION TAG	UNP Q99104
B	1450	HIS	-	EXPRESSION TAG	UNP Q99104
B	1451	HIS	-	EXPRESSION TAG	UNP Q99104
B	1452	HIS	-	EXPRESSION TAG	UNP Q99104
B	1453	HIS	-	EXPRESSION TAG	UNP Q99104
B	1454	HIS	-	EXPRESSION TAG	UNP Q99104
B	1455	HIS	-	EXPRESSION TAG	UNP Q99104
B	1456	SER	-	EXPRESSION TAG	UNP Q99104
B	1457	SER	-	EXPRESSION TAG	UNP Q99104
B	1458	GLY	-	EXPRESSION TAG	UNP Q99104
B	1459	LEU	-	EXPRESSION TAG	UNP Q99104
B	1460	GLY	-	EXPRESSION TAG	UNP Q99104
B	1461	VAL	-	EXPRESSION TAG	UNP Q99104
B	1462	LEU	-	EXPRESSION TAG	UNP Q99104
B	1463	PHE	-	EXPRESSION TAG	UNP Q99104
B	1464	GLN	-	EXPRESSION TAG	UNP Q99104
B	1465	GLY	-	EXPRESSION TAG	UNP Q99104
B	1466	PRO	-	EXPRESSION TAG	UNP Q99104
B	1467	GLY	-	EXPRESSION TAG	UNP Q99104
B	1468	SER	-	EXPRESSION TAG	UNP Q99104
C	1450	HIS	-	EXPRESSION TAG	UNP Q99104
C	1451	HIS	-	EXPRESSION TAG	UNP Q99104
C	1452	HIS	-	EXPRESSION TAG	UNP Q99104
C	1453	HIS	-	EXPRESSION TAG	UNP Q99104
C	1454	HIS	-	EXPRESSION TAG	UNP Q99104
C	1455	HIS	-	EXPRESSION TAG	UNP Q99104
C	1456	SER	-	EXPRESSION TAG	UNP Q99104
C	1457	SER	-	EXPRESSION TAG	UNP Q99104
C	1458	GLY	-	EXPRESSION TAG	UNP Q99104
C	1459	LEU	-	EXPRESSION TAG	UNP Q99104
C	1460	GLY	-	EXPRESSION TAG	UNP Q99104
C	1461	VAL	-	EXPRESSION TAG	UNP Q99104
C	1462	LEU	-	EXPRESSION TAG	UNP Q99104
C	1463	PHE	-	EXPRESSION TAG	UNP Q99104
C	1464	GLN	-	EXPRESSION TAG	UNP Q99104
C	1465	GLY	-	EXPRESSION TAG	UNP Q99104
C	1466	PRO	-	EXPRESSION TAG	UNP Q99104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1467	GLY	-	EXPRESSION TAG	UNP Q99104
C	1468	SER	-	EXPRESSION TAG	UNP Q99104
D	1450	HIS	-	EXPRESSION TAG	UNP Q99104
D	1451	HIS	-	EXPRESSION TAG	UNP Q99104
D	1452	HIS	-	EXPRESSION TAG	UNP Q99104
D	1453	HIS	-	EXPRESSION TAG	UNP Q99104
D	1454	HIS	-	EXPRESSION TAG	UNP Q99104
D	1455	HIS	-	EXPRESSION TAG	UNP Q99104
D	1456	SER	-	EXPRESSION TAG	UNP Q99104
D	1457	SER	-	EXPRESSION TAG	UNP Q99104
D	1458	GLY	-	EXPRESSION TAG	UNP Q99104
D	1459	LEU	-	EXPRESSION TAG	UNP Q99104
D	1460	GLY	-	EXPRESSION TAG	UNP Q99104
D	1461	VAL	-	EXPRESSION TAG	UNP Q99104
D	1462	LEU	-	EXPRESSION TAG	UNP Q99104
D	1463	PHE	-	EXPRESSION TAG	UNP Q99104
D	1464	GLN	-	EXPRESSION TAG	UNP Q99104
D	1465	GLY	-	EXPRESSION TAG	UNP Q99104
D	1466	PRO	-	EXPRESSION TAG	UNP Q99104
D	1467	GLY	-	EXPRESSION TAG	UNP Q99104
D	1468	SER	-	EXPRESSION TAG	UNP Q99104
E	1450	HIS	-	EXPRESSION TAG	UNP Q99104
E	1451	HIS	-	EXPRESSION TAG	UNP Q99104
E	1452	HIS	-	EXPRESSION TAG	UNP Q99104
E	1453	HIS	-	EXPRESSION TAG	UNP Q99104
E	1454	HIS	-	EXPRESSION TAG	UNP Q99104
E	1455	HIS	-	EXPRESSION TAG	UNP Q99104
E	1456	SER	-	EXPRESSION TAG	UNP Q99104
E	1457	SER	-	EXPRESSION TAG	UNP Q99104
E	1458	GLY	-	EXPRESSION TAG	UNP Q99104
E	1459	LEU	-	EXPRESSION TAG	UNP Q99104
E	1460	GLY	-	EXPRESSION TAG	UNP Q99104
E	1461	VAL	-	EXPRESSION TAG	UNP Q99104
E	1462	LEU	-	EXPRESSION TAG	UNP Q99104
E	1463	PHE	-	EXPRESSION TAG	UNP Q99104
E	1464	GLN	-	EXPRESSION TAG	UNP Q99104
E	1465	GLY	-	EXPRESSION TAG	UNP Q99104
E	1466	PRO	-	EXPRESSION TAG	UNP Q99104
E	1467	GLY	-	EXPRESSION TAG	UNP Q99104
E	1468	SER	-	EXPRESSION TAG	UNP Q99104
F	1450	HIS	-	EXPRESSION TAG	UNP Q99104
F	1451	HIS	-	EXPRESSION TAG	UNP Q99104

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1452	HIS	-	EXPRESSION TAG	UNP Q99104
F	1453	HIS	-	EXPRESSION TAG	UNP Q99104
F	1454	HIS	-	EXPRESSION TAG	UNP Q99104
F	1455	HIS	-	EXPRESSION TAG	UNP Q99104
F	1456	SER	-	EXPRESSION TAG	UNP Q99104
F	1457	SER	-	EXPRESSION TAG	UNP Q99104
F	1458	GLY	-	EXPRESSION TAG	UNP Q99104
F	1459	LEU	-	EXPRESSION TAG	UNP Q99104
F	1460	GLY	-	EXPRESSION TAG	UNP Q99104
F	1461	VAL	-	EXPRESSION TAG	UNP Q99104
F	1462	LEU	-	EXPRESSION TAG	UNP Q99104
F	1463	PHE	-	EXPRESSION TAG	UNP Q99104
F	1464	GLN	-	EXPRESSION TAG	UNP Q99104
F	1465	GLY	-	EXPRESSION TAG	UNP Q99104
F	1466	PRO	-	EXPRESSION TAG	UNP Q99104
F	1467	GLY	-	EXPRESSION TAG	UNP Q99104
F	1468	SER	-	EXPRESSION TAG	UNP Q99104
G	1450	HIS	-	EXPRESSION TAG	UNP Q99104
G	1451	HIS	-	EXPRESSION TAG	UNP Q99104
G	1452	HIS	-	EXPRESSION TAG	UNP Q99104
G	1453	HIS	-	EXPRESSION TAG	UNP Q99104
G	1454	HIS	-	EXPRESSION TAG	UNP Q99104
G	1455	HIS	-	EXPRESSION TAG	UNP Q99104
G	1456	SER	-	EXPRESSION TAG	UNP Q99104
G	1457	SER	-	EXPRESSION TAG	UNP Q99104
G	1458	GLY	-	EXPRESSION TAG	UNP Q99104
G	1459	LEU	-	EXPRESSION TAG	UNP Q99104
G	1460	GLY	-	EXPRESSION TAG	UNP Q99104
G	1461	VAL	-	EXPRESSION TAG	UNP Q99104
G	1462	LEU	-	EXPRESSION TAG	UNP Q99104
G	1463	PHE	-	EXPRESSION TAG	UNP Q99104
G	1464	GLN	-	EXPRESSION TAG	UNP Q99104
G	1465	GLY	-	EXPRESSION TAG	UNP Q99104
G	1466	PRO	-	EXPRESSION TAG	UNP Q99104
G	1467	GLY	-	EXPRESSION TAG	UNP Q99104
G	1468	SER	-	EXPRESSION TAG	UNP Q99104
H	1450	HIS	-	EXPRESSION TAG	UNP Q99104
H	1451	HIS	-	EXPRESSION TAG	UNP Q99104
H	1452	HIS	-	EXPRESSION TAG	UNP Q99104
H	1453	HIS	-	EXPRESSION TAG	UNP Q99104
H	1454	HIS	-	EXPRESSION TAG	UNP Q99104
H	1455	HIS	-	EXPRESSION TAG	UNP Q99104

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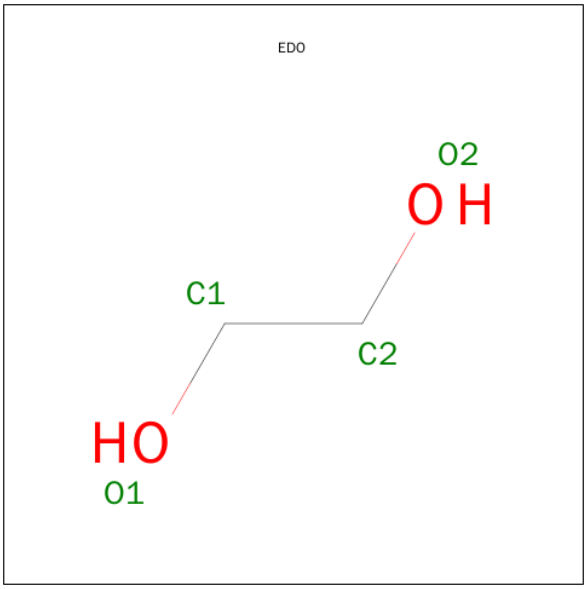
Chain	Residue	Modelled	Actual	Comment	Reference
H	1456	SER	-	EXPRESSION TAG	UNP Q99104
H	1457	SER	-	EXPRESSION TAG	UNP Q99104
H	1458	GLY	-	EXPRESSION TAG	UNP Q99104
H	1459	LEU	-	EXPRESSION TAG	UNP Q99104
H	1460	GLY	-	EXPRESSION TAG	UNP Q99104
H	1461	VAL	-	EXPRESSION TAG	UNP Q99104
H	1462	LEU	-	EXPRESSION TAG	UNP Q99104
H	1463	PHE	-	EXPRESSION TAG	UNP Q99104
H	1464	GLN	-	EXPRESSION TAG	UNP Q99104
H	1465	GLY	-	EXPRESSION TAG	UNP Q99104
H	1466	PRO	-	EXPRESSION TAG	UNP Q99104
H	1467	GLY	-	EXPRESSION TAG	UNP Q99104
H	1468	SER	-	EXPRESSION TAG	UNP Q99104

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	B	38	Total O 38 38	0	0

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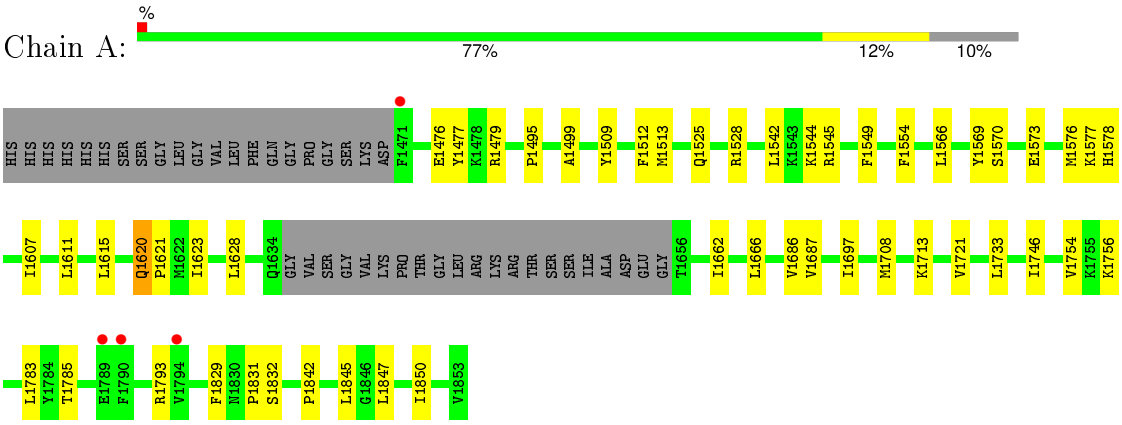
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	50	Total O 50 50	0	0
3	D	76	Total O 76 76	0	0
3	E	46	Total O 46 46	0	0
3	F	44	Total O 44 44	0	0
3	G	39	Total O 39 39	0	0
3	H	8	Total O 8 8	0	0

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.

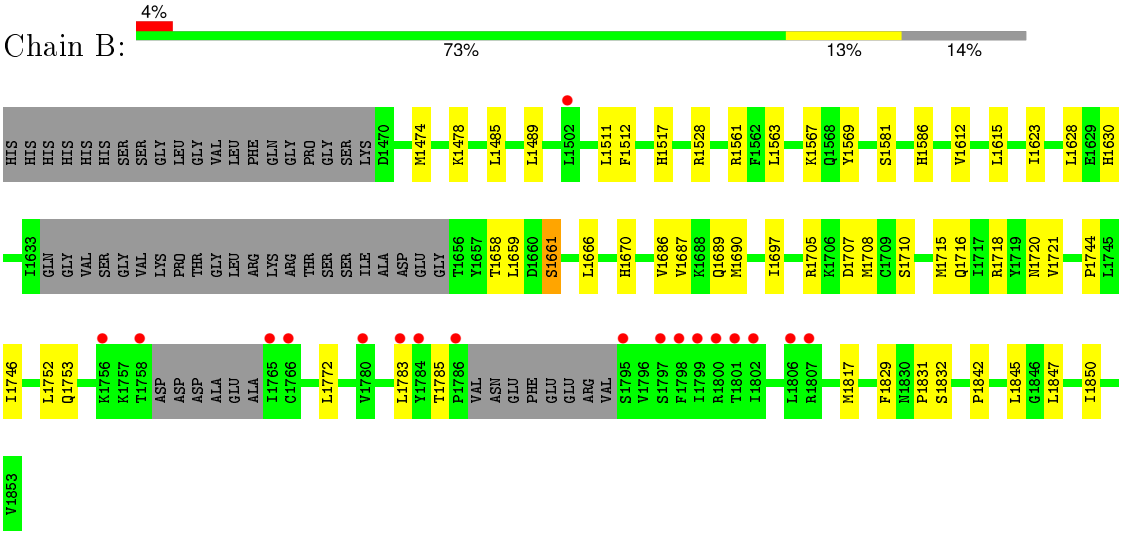
- Molecule 1: Unconventional myosin-Va

Chain A:



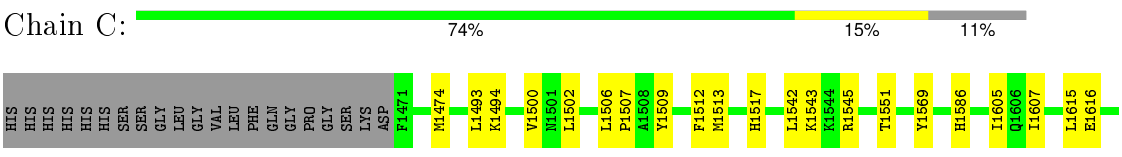
- Molecule 1: Unconventional myosin-Va

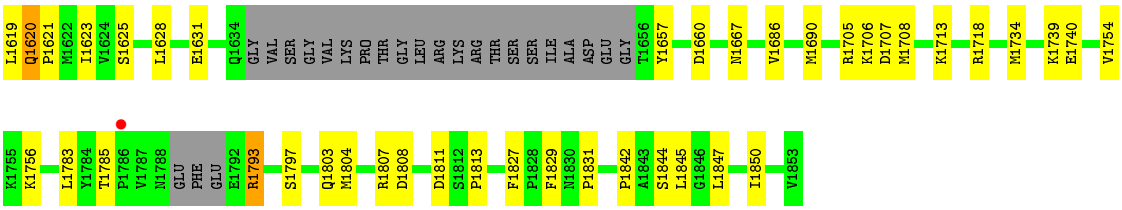
Chain B:



- Molecule 1: Unconventional myosin-Va

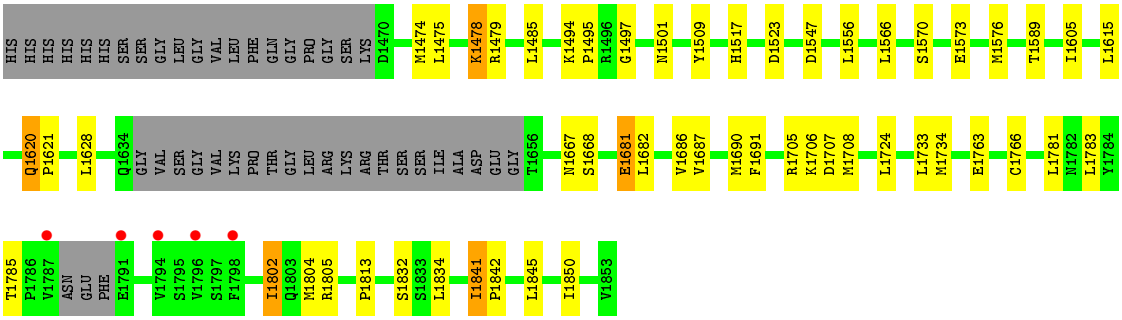
Chain C:





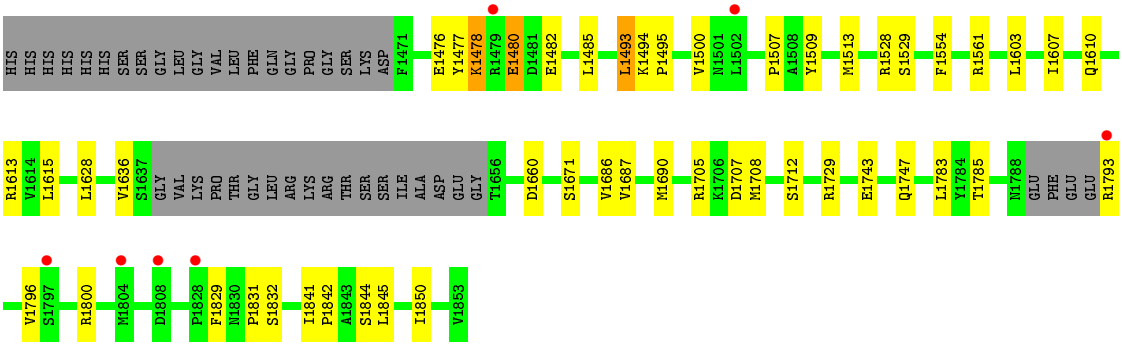
- Molecule 1: Unconventional myosin-Va

Chain D:



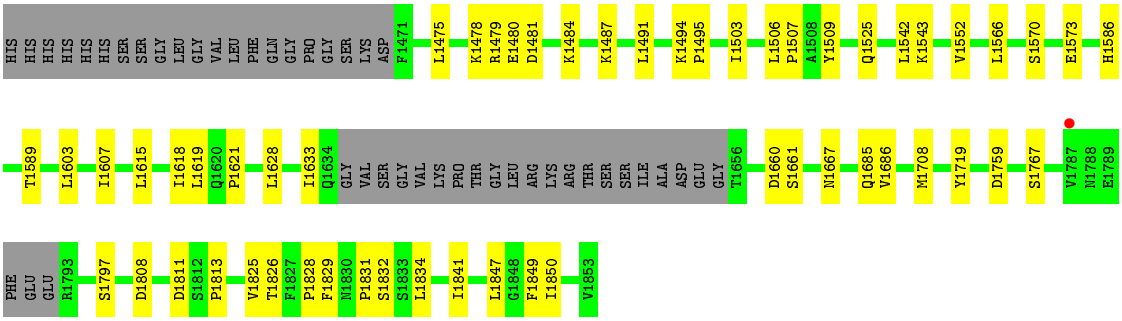
- Molecule 1: Unconventional myosin-Va

Chain E:



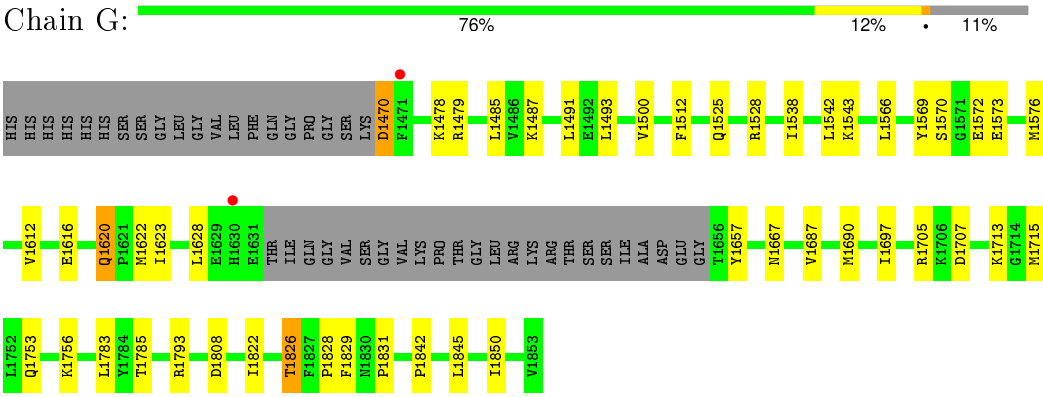
- Molecule 1: Unconventional myosin-Va

Chain F:



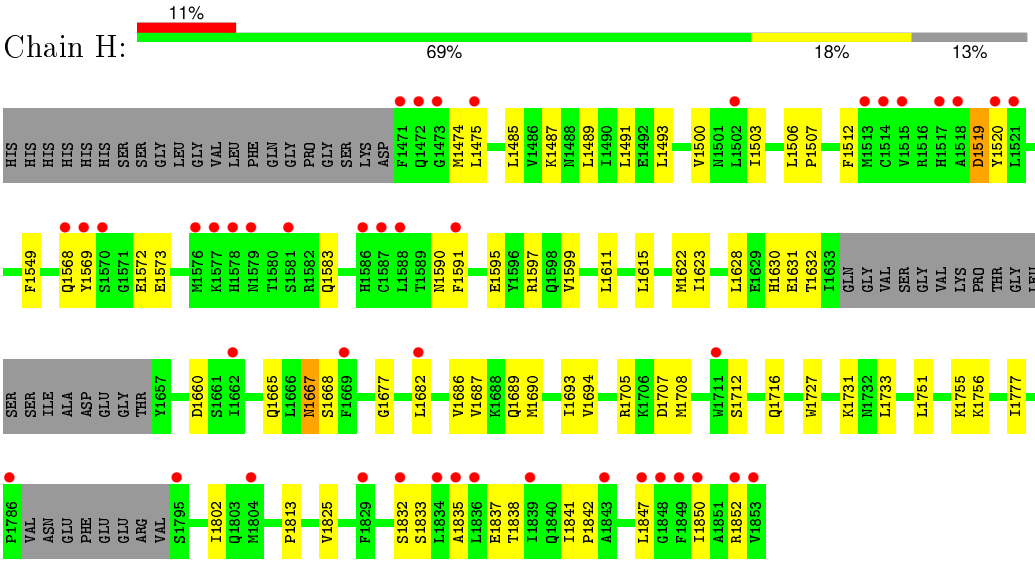
- Molecule 1: Unconventional myosin-Va

Chain G:



- Molecule 1: Unconventional myosin-Va

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.98Å 165.35Å 173.02Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	41.79 – 2.50 41.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (41.79-2.50) 98.4 (41.79-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.173 , 0.225 0.187 , 0.234	Depositor DCC
R_{free} test set	6651 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.4	EDS
Estimated twinning fraction	0.007 for -h,l,k 0.017 for -h,-l,-k 0.058 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	2 of 131820 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23277	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.32 % 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 7.1963e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: EDO

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	0.45	0/2962	0.56	0/3997
1	B	0.38	0/2785	0.52	0/3767
1	C	0.40	0/2940	0.54	0/3966
1	D	0.44	0/2922	0.58	0/3945
1	E	0.38	0/2929	0.53	0/3953
1	F	0.38	0/2920	0.53	0/3941
1	G	0.38	0/2956	0.53	0/3987
1	H	0.32	0/2795	0.48	0/3787
All	All	0.39	0/23209	0.53	0/31343

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

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	2913	0	2971	33	0
1	B	2740	0	2746	32	0
1	C	2890	0	2958	32	0
1	D	2876	0	2917	33	0
1	E	2883	0	2944	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2873	0	2930	28	0
1	G	2907	0	2966	28	0
1	H	2751	0	2733	41	0
2	A	16	0	24	0	0
2	B	8	0	12	1	0
2	C	12	0	18	0	0
2	D	12	0	18	1	0
2	E	8	0	12	0	0
2	F	12	0	18	0	0
2	G	12	0	18	0	0
2	H	8	0	12	1	0
3	A	55	0	0	0	0
3	B	38	0	0	4	0
3	C	50	0	0	1	0
3	D	76	0	0	1	0
3	E	46	0	0	0	0
3	F	44	0	0	2	0
3	G	39	0	0	0	0
3	H	8	0	0	0	0
All	All	23277	0	23297	248	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 (248) 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:1785:THR:HG22	1:E:1793:ARG:HH12	1.47	0.79
1:A:1479:ARG:HH21	1:A:1525:GLN:HG2	1.54	0.72
1:E:1687:VAL:HA	1:E:1690:MET:HE2	1.73	0.70
1:E:1493:LEU:HD21	1:E:1500:VAL:HG21	1.74	0.70
1:E:1485:LEU:HD13	1:E:1850:ILE:HD11	1.73	0.69
1:B:1630:HIS:O	1:B:1716:GLN:NE2	2.26	0.68
1:B:1705:ARG:NH2	1:B:1707:ASP:OD2	2.22	0.66
1:D:1706:LYS:HG2	1:D:1783:LEU:HD22	1.77	0.66
1:D:1605:ILE:HG23	2:D:1903:EDO:H22	1.78	0.64
1:G:1715:MET:SD	1:G:1753:GLN:NE2	2.67	0.63
1:F:1847:LEU:HB3	1:F:1850:ILE:HD12	1.81	0.63
1:G:1479:ARG:NH1	1:G:1525:GLN:OE1	2.32	0.62
1:B:1847:LEU:HB3	1:B:1850:ILE:HD12	1.83	0.61
1:E:1842:PRO:HG2	1:E:1845:LEU:HG	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1847:LEU:HB3	1:H:1850:ILE:HD12	1.82	0.60
1:A:1754:VAL:O	1:A:1756:LYS:NZ	2.34	0.60
1:H:1493:LEU:HD21	1:H:1500:VAL:HG11	1.83	0.59
1:D:1687:VAL:HA	1:D:1690:MET:HE2	1.83	0.59
1:H:1615:LEU:HD13	1:H:1690:MET:HG2	1.83	0.59
1:B:1666:LEU:HD22	1:B:1690:MET:HE3	1.84	0.58
1:H:1485:LEU:HD13	1:H:1850:ILE:HD11	1.84	0.58
1:D:1497:GLY:O	1:D:1501:ASN:ND2	2.35	0.58
1:B:1628:LEU:HB3	1:B:1708:MET:HE1	1.83	0.58
1:B:1485:LEU:HD13	1:B:1850:ILE:HD11	1.84	0.58
1:C:1705:ARG:HB3	1:C:1707:ASP:OD1	2.04	0.57
1:G:1829:PHE:CE2	1:G:1831:PRO:HG3	2.39	0.57
1:H:1623:ILE:HD13	1:H:1694:VAL:HA	1.87	0.57
1:C:1847:LEU:HB3	1:C:1850:ILE:HD12	1.85	0.57
1:C:1829:PHE:CE2	1:C:1831:PRO:HG3	2.40	0.56
1:G:1783:LEU:O	1:G:1785:THR:HG23	2.05	0.56
1:A:1783:LEU:O	1:A:1785:THR:HG23	2.05	0.56
1:G:1842:PRO:HG2	1:G:1845:LEU:HG	1.87	0.56
1:A:1829:PHE:CE2	1:A:1831:PRO:HG3	2.41	0.55
1:B:1623:ILE:HD12	1:B:1697:ILE:HD12	1.87	0.55
1:H:1630:HIS:O	1:H:1716:GLN:NE2	2.40	0.55
1:A:1628:LEU:HB3	1:A:1708:MET:HE1	1.87	0.55
1:D:1628:LEU:HD22	1:D:1708:MET:HE2	1.89	0.55
1:G:1612:VAL:HG11	1:G:1822:ILE:HG12	1.88	0.54
1:G:1628:LEU:O	1:G:1713:LYS:NZ	2.26	0.54
1:H:1622:MET:SD	1:H:1665:GLN:HG3	2.48	0.54
1:G:1705:ARG:HB3	1:G:1707:ASP:OD1	2.08	0.54
1:B:1489:LEU:HD13	1:B:1511:LEU:HG	1.90	0.53
1:B:1721:VAL:HG11	1:B:1746:ILE:HD11	1.90	0.53
1:C:1754:VAL:O	1:C:1756:LYS:NZ	2.41	0.53
1:D:1573:GLU:HA	1:D:1576:MET:CE	2.38	0.53
1:B:1586:HIS:HD2	3:B:2002:HOH:O	1.91	0.53
1:H:1677:GLY:HA3	2:H:1902:EDO:H21	1.91	0.53
1:E:1509:TYR:O	1:E:1513:MET:HG3	2.08	0.53
1:D:1478:LYS:H	1:D:1478:LYS:HD2	1.73	0.52
1:H:1503:ILE:O	1:H:1506:LEU:HB2	2.09	0.52
1:B:1829:PHE:CE2	1:B:1831:PRO:HG3	2.45	0.52
1:G:1623:ILE:HD12	1:G:1697:ILE:HD12	1.92	0.51
1:H:1835:ALA:O	1:H:1838:THR:OG1	2.27	0.51
1:A:1687:VAL:HG11	1:A:1733:LEU:HD13	1.93	0.50
1:C:1842:PRO:HG2	1:C:1845:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1721:VAL:HG11	1:A:1746:ILE:HD11	1.94	0.50
1:G:1478:LYS:HD2	1:G:1478:LYS:N	2.27	0.50
1:G:1512:PHE:CZ	1:G:1569:TYR:HB2	2.45	0.50
1:C:1628:LEU:HD13	1:C:1708:MET:HE2	1.94	0.50
1:A:1620:GLN:HA	1:A:1623:ILE:HD12	1.93	0.50
1:E:1561:ARG:NH1	1:E:1832:SER:HB2	2.27	0.50
1:C:1542:LEU:CD1	1:C:1607:ILE:HG12	2.42	0.49
1:E:1628:LEU:HB3	1:E:1708:MET:CE	2.43	0.49
1:A:1623:ILE:HD13	1:A:1697:ILE:HD12	1.95	0.49
1:E:1482:GLU:OE1	1:E:1529:SER:OG	2.29	0.49
1:C:1616:GLU:O	1:C:1620:GLN:HB3	2.12	0.49
1:G:1487:LYS:HA	1:G:1491:LEU:HB2	1.95	0.49
1:D:1573:GLU:HA	1:D:1576:MET:HE3	1.95	0.49
1:D:1763:GLU:HG2	1:D:1805:ARG:NH2	2.27	0.49
1:D:1478:LYS:N	1:D:1478:LYS:HD2	2.27	0.49
1:E:1478:LYS:N	1:E:1478:LYS:HD2	2.28	0.49
1:H:1519:ASP:O	1:H:1590:ASN:ND2	2.46	0.49
1:E:1796:VAL:O	1:E:1800:ARG:HG2	2.13	0.48
1:F:1509:TYR:CE1	1:F:1834:LEU:HD23	2.48	0.48
1:D:1475:LEU:HD11	1:D:1841:ILE:HD11	1.95	0.48
1:H:1475:LEU:HD22	1:H:1850:ILE:HG22	1.96	0.48
1:D:1566:LEU:O	1:D:1570:SER:HB3	2.12	0.48
1:B:1718:ARG:HD3	1:B:1753:GLN:OE1	2.14	0.48
1:F:1586:HIS:HD2	3:F:2033:HOH:O	1.96	0.48
1:A:1577:LYS:HG2	1:A:1578:HIS:CE1	2.48	0.48
1:F:1542:LEU:HD22	1:F:1552:VAL:HG22	1.95	0.48
1:A:1785:THR:HG22	1:A:1793:ARG:NH2	2.29	0.48
1:C:1509:TYR:O	1:C:1513:MET:HG3	2.13	0.48
1:C:1586:HIS:HD2	3:C:2034:HOH:O	1.96	0.48
1:B:1783:LEU:O	1:B:1785:THR:HG23	2.13	0.48
1:A:1628:LEU:HB3	1:A:1708:MET:CE	2.44	0.48
1:F:1826:THR:O	1:F:1828:PRO:HD3	2.14	0.48
1:F:1573:GLU:CD	1:F:1573:GLU:H	2.17	0.47
1:G:1470:ASP:OD1	1:G:1470:ASP:N	2.46	0.47
1:B:1842:PRO:HG2	1:B:1845:LEU:HG	1.95	0.47
1:H:1705:ARG:HB3	1:H:1707:ASP:OD1	2.14	0.47
1:F:1618:ILE:O	1:F:1621:PRO:HD2	2.14	0.47
1:D:1766:CYS:SG	1:D:1805:ARG:HG2	2.54	0.47
1:G:1485:LEU:HD13	1:G:1850:ILE:HD11	1.97	0.47
1:E:1615:LEU:HD11	1:E:1686:VAL:HG13	1.96	0.47
1:C:1620:GLN:HG3	1:C:1621:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1658:THR:H	1:B:1661:SER:HB2	1.80	0.47
1:B:1474:MET:HB3	1:B:1517:HIS:HB2	1.97	0.47
1:E:1603:LEU:O	1:E:1607:ILE:HG13	2.15	0.47
1:E:1480:GLU:HG3	1:E:1480:GLU:H	1.39	0.47
1:D:1615:LEU:HD11	1:D:1686:VAL:HG13	1.96	0.47
1:D:1509:TYR:CE1	1:D:1834:LEU:HD23	2.49	0.47
1:A:1615:LEU:HD11	1:A:1686:VAL:HG13	1.97	0.47
1:D:1628:LEU:HB3	1:D:1708:MET:CE	2.45	0.47
1:B:1628:LEU:HB3	1:B:1708:MET:CE	2.45	0.46
1:A:1509:TYR:O	1:A:1513:MET:HG3	2.15	0.46
1:H:1527:VAL:O	1:H:1531:LEU:HG	2.15	0.46
1:B:1689:GLN:NE2	3:B:2038:HOH:O	2.47	0.46
1:C:1706:LYS:HG2	1:C:1783:LEU:HD22	1.97	0.46
1:H:1506:LEU:HB3	1:H:1507:PRO:HD3	1.98	0.46
1:G:1538:ILE:O	1:G:1542:LEU:HG	2.15	0.46
1:C:1605:ILE:HG13	1:C:1827:PHE:HE2	1.81	0.46
1:G:1566:LEU:O	1:G:1570:SER:HB3	2.16	0.46
1:B:1744:PRO:O	1:B:1772:LEU:HD21	2.15	0.46
1:F:1480:GLU:CD	1:F:1480:GLU:H	2.19	0.46
1:C:1545:ARG:HB2	1:C:1551:THR:HG21	1.98	0.46
1:D:1494:LYS:HA	1:D:1495:PRO:HD2	1.83	0.46
1:C:1615:LEU:HD11	1:C:1686:VAL:HG13	1.97	0.46
1:G:1687:VAL:HA	1:G:1690:MET:HE2	1.97	0.46
1:H:1689:GLN:O	1:H:1693:ILE:HG13	2.16	0.46
1:G:1622:MET:HG2	1:G:1657:TYR:CD2	2.51	0.46
1:A:1528:ARG:HD3	1:C:1813:PRO:O	2.15	0.46
1:E:1610:GLN:OE1	1:E:1613:ARG:NH1	2.48	0.46
1:B:1512:PHE:CZ	1:B:1569:TYR:HB2	2.51	0.46
1:A:1545:ARG:NH1	1:G:1808:ASP:HB3	2.32	0.45
1:A:1566:LEU:O	1:A:1570:SER:HB3	2.15	0.45
1:F:1829:PHE:CE2	1:F:1831:PRO:HG3	2.50	0.45
1:B:1612:VAL:HA	1:B:1615:LEU:HD12	1.98	0.45
1:G:1542:LEU:HD11	1:G:1607:ILE:HG12	1.98	0.45
1:C:1619:LEU:HB3	1:C:1623:ILE:HD11	1.99	0.45
1:D:1474:MET:HB3	1:D:1517:HIS:HB2	1.99	0.45
1:D:1620:GLN:HG3	1:D:1621:PRO:HD3	1.99	0.45
1:F:1487:LYS:HA	1:F:1491:LEU:HB2	1.98	0.45
1:H:1667:ASN:CG	1:H:1731:LYS:HZ1	2.20	0.45
1:A:1620:GLN:HG3	1:A:1621:PRO:HD3	1.99	0.45
1:C:1615:LEU:HD13	1:C:1690:MET:HG2	1.99	0.45
1:F:1685:GLN:CD	1:F:1825:VAL:HG23	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1615:LEU:HD11	1:F:1686:VAL:HG13	1.97	0.45
1:B:1612:VAL:O	1:B:1615:LEU:HB2	2.17	0.45
1:A:1549:PHE:CE1	1:A:1611:LEU:HD11	2.52	0.45
1:C:1474:MET:HB3	1:C:1517:HIS:HB2	1.98	0.45
1:H:1572:GLU:OE2	1:H:1597:ARG:NH1	2.50	0.45
1:F:1633:ILE:HD11	1:F:1719:TYR:CD1	2.52	0.45
1:H:1631:GLU:HG3	1:H:1716:GLN:OE1	2.17	0.45
1:F:1478:LYS:O	1:F:1481:ASP:HB2	2.17	0.45
1:D:1485:LEU:HD13	1:D:1850:ILE:HD11	2.00	0.44
1:C:1625:SER:OG	1:C:1657:TYR:O	2.31	0.44
1:H:1781:LEU:HD11	1:H:1802:ILE:HD12	2.00	0.44
1:H:1595:GLU:O	1:H:1599:VAL:HG23	2.17	0.44
1:E:1783:LEU:O	1:E:1785:THR:HG23	2.18	0.44
1:D:1763:GLU:HG2	1:D:1805:ARG:CZ	2.48	0.44
1:E:1500:VAL:HG22	1:E:1507:PRO:HD3	1.99	0.44
1:A:1542:LEU:HD13	1:A:1607:ILE:HG12	2.00	0.44
1:D:1687:VAL:HG11	1:D:1733:LEU:HD13	1.99	0.44
1:F:1566:LEU:O	1:F:1570:SER:HB3	2.18	0.44
1:F:1685:GLN:OE1	1:F:1825:VAL:HG23	2.17	0.44
1:A:1573:GLU:HA	1:A:1576:MET:HG3	1.99	0.44
1:G:1493:LEU:HD21	1:G:1500:VAL:HG21	2.00	0.44
1:G:1785:THR:HG22	1:G:1793:ARG:NH2	2.33	0.44
1:G:1573:GLU:HA	1:G:1576:MET:HE2	2.00	0.44
1:H:1686:VAL:O	1:H:1690:MET:HG3	2.17	0.43
1:G:1572:GLU:OE2	1:G:1597:ARG:NH1	2.51	0.43
1:E:1495:PRO:HB3	1:E:1554:PHE:CG	2.54	0.43
1:B:1615:LEU:HD11	1:B:1686:VAL:HG13	2.00	0.43
1:F:1829:PHE:CZ	1:F:1831:PRO:HG3	2.53	0.43
1:H:1474:MET:HE1	1:H:1520:TYR:CD1	2.53	0.43
1:C:1740:GLU:OE1	1:C:1740:GLU:N	2.51	0.43
1:C:1734:MET:HE3	1:C:1739:LYS:HE2	2.00	0.43
1:D:1479:ARG:NH2	1:D:1523:ASP:OD1	2.51	0.43
1:F:1475:LEU:HD11	1:F:1841:ILE:HD11	2.00	0.43
1:F:1506:LEU:HB3	1:F:1507:PRO:HD3	1.99	0.43
1:B:1659:LEU:HD22	1:B:1720:ASN:OD1	2.19	0.43
1:D:1842:PRO:HG2	1:D:1845:LEU:HG	2.00	0.43
1:B:1561:ARG:HB2	2:B:1902:EDO:H22	2.00	0.43
1:G:1826:THR:O	1:G:1828:PRO:HD3	2.19	0.43
1:H:1751:LEU:O	1:H:1756:LYS:HE3	2.18	0.43
1:A:1512:PHE:CZ	1:A:1569:TYR:HB2	2.54	0.43
1:C:1713:LYS:HA	1:C:1713:LYS:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1628:LEU:O	1:A:1713:LYS:NZ	2.42	0.42
1:A:1842:PRO:HG2	1:A:1845:LEU:HG	1.99	0.42
1:D:1781:LEU:HD11	1:D:1802:ILE:HD12	2.00	0.42
1:E:1528:ARG:HD3	1:F:1813:PRO:O	2.19	0.42
1:E:1743:GLU:O	1:E:1747:GLN:HG3	2.18	0.42
1:A:1495:PRO:HB3	1:A:1554:PHE:CG	2.54	0.42
1:F:1484:LYS:HE2	1:F:1849:PHE:CE1	2.55	0.42
1:A:1628:LEU:HD22	1:A:1708:MET:HE2	2.02	0.42
1:B:1528:ARG:HD3	1:H:1813:PRO:O	2.19	0.42
1:F:1603:LEU:O	1:F:1607:ILE:HG13	2.20	0.42
1:H:1549:PHE:CE1	1:H:1611:LEU:HD11	2.54	0.42
1:A:1479:ARG:NH2	1:A:1525:GLN:HG2	2.28	0.42
1:H:1489:LEU:HD11	1:H:1507:PRO:HA	2.02	0.42
1:C:1512:PHE:CZ	1:C:1569:TYR:HB2	2.55	0.42
1:F:1479:ARG:NH2	1:F:1525:GLN:HG2	2.34	0.42
1:H:1568:GLN:NE2	1:H:1832:SER:O	2.50	0.42
1:C:1506:LEU:HB3	1:C:1507:PRO:HD3	2.01	0.42
1:D:1705:ARG:HB3	1:D:1707:ASP:OD1	2.20	0.42
1:E:1707:ASP:OD1	1:E:1707:ASP:N	2.52	0.42
1:B:1670:HIS:HD2	3:B:2005:HOH:O	2.02	0.42
1:E:1476:GLU:HG2	1:E:1477:TYR:N	2.33	0.42
1:C:1493:LEU:HD21	1:C:1500:VAL:HG11	2.00	0.42
1:D:1681:GLU:HB2	3:D:2056:HOH:O	2.18	0.42
1:H:1573:GLU:H	1:H:1573:GLU:HG3	1.63	0.42
1:H:1841:ILE:HA	1:H:1842:PRO:HD2	1.83	0.42
1:G:1751:LEU:O	1:G:1756:LYS:HE3	2.20	0.42
1:H:1628:LEU:HD13	1:H:1708:MET:HE2	2.02	0.42
1:D:1556:LEU:HD21	1:D:1682:LEU:HD21	2.02	0.42
1:D:1783:LEU:O	1:D:1785:THR:HG23	2.20	0.41
1:C:1739:LYS:HE3	1:C:1739:LYS:HB2	1.96	0.41
1:A:1662:ILE:O	1:A:1666:LEU:HG	2.19	0.41
1:H:1583:GLN:HE22	1:H:1833:SER:HA	1.84	0.41
1:C:1803:GLN:O	1:C:1807[B]:ARG:HG2	2.20	0.41
1:F:1628:LEU:HD13	1:F:1708:MET:HE2	2.02	0.41
1:H:1755:LYS:HB2	1:H:1755:LYS:HE3	1.81	0.41
1:H:1682:LEU:HA	1:H:1682:LEU:HD12	1.93	0.41
1:D:1813:PRO:O	1:G:1528:ARG:HD3	2.21	0.41
1:D:1547:ASP:OD1	1:D:1547:ASP:N	2.42	0.41
1:E:1494:LYS:HA	1:E:1495:PRO:HD2	1.94	0.41
1:B:1687:VAL:HA	1:B:1690:MET:HE2	2.03	0.41
1:H:1727:TRP:O	1:H:1731:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1715:MET:SD	1:B:1753:GLN:NE2	2.83	0.41
1:E:1829:PHE:CE2	1:E:1831:PRO:HG3	2.56	0.41
1:A:1476:GLU:HG2	1:A:1477:TYR:N	2.36	0.41
1:F:1503:ILE:HD12	3:F:2007:HOH:O	2.19	0.41
1:A:1544:LYS:HE2	1:D:1589:THR:O	2.20	0.41
1:H:1475:LEU:HD23	1:H:1852:ARG:HA	2.03	0.41
1:F:1628:LEU:HB3	1:F:1708:MET:CE	2.51	0.41
1:B:1710:SER:O	1:B:1752:LEU:HB3	2.21	0.41
1:B:1563:LEU:O	1:B:1567:LYS:HG3	2.21	0.41
1:F:1619:LEU:HA	1:F:1619:LEU:HD23	1.88	0.41
1:H:1687:VAL:HG21	1:H:1733:LEU:HD13	2.03	0.41
1:G:1616:GLU:O	1:G:1620:GLN:HB3	2.20	0.41
1:H:1512:PHE:CZ	1:H:1569:TYR:HB2	2.55	0.41
1:A:1713:LYS:HA	1:A:1713:LYS:HD3	1.82	0.40
1:C:1734:MET:CE	1:C:1739:LYS:HE2	2.51	0.40
1:C:1785:THR:HG22	1:C:1793:ARG:HH21	1.87	0.40
1:H:1527:VAL:HG21	1:H:1591:PHE:CE2	2.56	0.40
1:E:1705:ARG:HB3	1:E:1707:ASP:OD1	2.21	0.40
1:F:1494:LYS:HA	1:F:1495:PRO:HD2	1.91	0.40
1:A:1847:LEU:O	1:A:1850:ILE:HG12	2.21	0.40
1:E:1690:MET:HB2	1:E:1690:MET:HE2	1.93	0.40
1:C:1686:VAL:O	1:C:1690:MET:HG3	2.20	0.40
1:C:1543:LYS:HB2	1:C:1543:LYS:HE2	1.86	0.40
1:D:1691:PHE:CE2	1:D:1724:LEU:HB3	2.56	0.40
1:E:1841:ILE:HA	1:E:1842:PRO:HD2	1.90	0.40
1:H:1777:ILE:O	1:H:1781:LEU:HG	2.22	0.40
1:A:1499:ALA:HB1	1:A:1842:PRO:HG3	2.04	0.40
1:B:1567:LYS:NZ	3:B:2018:HOH:O	2.51	0.40
1:H:1487:LYS:HA	1:H:1491:LEU:HD12	2.03	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	358/404 (89%)	354 (99%)	4 (1%)	0	100	100
1	B	340/404 (84%)	325 (96%)	15 (4%)	0	100	100
1	C	354/404 (88%)	347 (98%)	7 (2%)	0	100	100
1	D	354/404 (88%)	343 (97%)	11 (3%)	0	100	100
1	E	355/404 (88%)	347 (98%)	8 (2%)	0	100	100
1	F	353/404 (87%)	347 (98%)	6 (2%)	0	100	100
1	G	356/404 (88%)	348 (98%)	8 (2%)	0	100	100
1	H	346/404 (86%)	331 (96%)	15 (4%)	0	100	100
All	All	2816/3232 (87%)	2742 (97%)	74 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/365 (90%)	328 (99%)	2 (1%)	90	97
1	B	305/365 (84%)	300 (98%)	5 (2%)	70	90
1	C	327/365 (90%)	314 (96%)	13 (4%)	38	64
1	D	324/365 (89%)	314 (97%)	10 (3%)	47	75
1	E	326/365 (89%)	317 (97%)	9 (3%)	51	78
1	F	324/365 (89%)	313 (97%)	11 (3%)	44	72
1	G	330/365 (90%)	324 (98%)	6 (2%)	66	88
1	H	303/365 (83%)	294 (97%)	9 (3%)	48	76
All	All	2569/2920 (88%)	2504 (98%)	65 (2%)	55	82

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1620	GLN
1	A	1832	SER

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Mol	Chain	Res	Type
1	B	1478	LYS
1	B	1581	SER
1	B	1661	SER
1	B	1817	MET
1	B	1832	SER
1	C	1494	LYS
1	C	1502	LEU
1	C	1620	GLN
1	C	1631	GLU
1	C	1660	ASP
1	C	1667	ASN
1	C	1718	ARG
1	C	1793	ARG
1	C	1797	SER
1	C	1804	MET
1	C	1808	ASP
1	C	1811	ASP
1	C	1844	SER
1	D	1478	LYS
1	D	1620	GLN
1	D	1667	ASN
1	D	1668	SER
1	D	1681	GLU
1	D	1734	MET
1	D	1802	ILE
1	D	1804	MET
1	D	1832	SER
1	D	1841	ILE
1	E	1478	LYS
1	E	1480	GLU
1	E	1493	LEU
1	E	1636	VAL
1	E	1660	ASP
1	E	1671	SER
1	E	1712	SER
1	E	1729	ARG
1	E	1844	SER
1	F	1543	LYS
1	F	1589	THR
1	F	1660	ASP
1	F	1661	SER
1	F	1667	ASN

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Mol	Chain	Res	Type
1	F	1759	ASP
1	F	1767	SER
1	F	1797	SER
1	F	1808	ASP
1	F	1811	ASP
1	F	1832	SER
1	G	1470	ASP
1	G	1543	LYS
1	G	1620	GLN
1	G	1667	ASN
1	G	1718	ARG
1	G	1826	THR
1	H	1519	ASP
1	H	1528	ARG
1	H	1632	THR
1	H	1660	ASP
1	H	1667	ASN
1	H	1668	SER
1	H	1712	SER
1	H	1825	VAL
1	H	1837	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1586	HIS
1	B	1689	GLN
1	C	1716	GLN
1	F	1525	GLN
1	F	1617	ASN
1	H	1814	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

22 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	EDO	A	1901	-	3,3,3	0.65	0	2,2,2	0.07	0
2	EDO	A	1902	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	A	1903	-	3,3,3	0.54	0	2,2,2	0.47	0
2	EDO	A	1904	-	3,3,3	0.40	0	2,2,2	0.48	0
2	EDO	B	1901	-	3,3,3	0.46	0	2,2,2	0.44	0
2	EDO	B	1902	-	3,3,3	0.43	0	2,2,2	0.51	0
2	EDO	C	1901	-	3,3,3	0.52	0	2,2,2	0.63	0
2	EDO	C	1902	-	3,3,3	0.40	0	2,2,2	0.53	0
2	EDO	C	1903	-	3,3,3	0.47	0	2,2,2	0.43	0
2	EDO	D	1901	-	3,3,3	0.51	0	2,2,2	0.37	0
2	EDO	D	1902	-	3,3,3	0.46	0	2,2,2	0.50	0
2	EDO	D	1903	-	3,3,3	0.43	0	2,2,2	0.49	0
2	EDO	E	1901	-	3,3,3	0.52	0	2,2,2	0.31	0
2	EDO	E	1902	-	3,3,3	0.47	0	2,2,2	0.48	0
2	EDO	F	1901	-	3,3,3	0.58	0	2,2,2	0.26	0
2	EDO	F	1902	-	3,3,3	0.46	0	2,2,2	0.60	0
2	EDO	F	1903	-	3,3,3	0.39	0	2,2,2	0.53	0
2	EDO	G	1901	-	3,3,3	0.56	0	2,2,2	0.47	0
2	EDO	G	1902	-	3,3,3	0.50	0	2,2,2	0.32	0
2	EDO	G	1903	-	3,3,3	0.48	0	2,2,2	0.36	0
2	EDO	H	1901	-	3,3,3	0.49	0	2,2,2	0.45	0
2	EDO	H	1902	-	3,3,3	0.46	0	2,2,2	0.39	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	EDO	A	1901	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1902	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1903	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1904	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1901	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1902	-	-	0/1/1/1	0/0/0/0
2	EDO	C	1901	-	-	0/1/1/1	0/0/0/0
2	EDO	C	1902	-	-	0/1/1/1	0/0/0/0
2	EDO	C	1903	-	-	0/1/1/1	0/0/0/0
2	EDO	D	1901	-	-	0/1/1/1	0/0/0/0
2	EDO	D	1902	-	-	0/1/1/1	0/0/0/0
2	EDO	D	1903	-	-	0/1/1/1	0/0/0/0
2	EDO	E	1901	-	-	0/1/1/1	0/0/0/0
2	EDO	E	1902	-	-	0/1/1/1	0/0/0/0
2	EDO	F	1901	-	-	0/1/1/1	0/0/0/0
2	EDO	F	1902	-	-	0/1/1/1	0/0/0/0
2	EDO	F	1903	-	-	0/1/1/1	0/0/0/0
2	EDO	G	1901	-	-	0/1/1/1	0/0/0/0
2	EDO	G	1902	-	-	0/1/1/1	0/0/0/0
2	EDO	G	1903	-	-	0/1/1/1	0/0/0/0
2	EDO	H	1901	-	-	0/1/1/1	0/0/0/0
2	EDO	H	1902	-	-	0/1/1/1	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1902	EDO	1	0
2	D	1903	EDO	1	0
2	H	1902	EDO	1	0

5.7 Other polymers (i)

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	362/404 (89%)	-0.22	4 (1%) 82 84	28, 47, 80, 125	0
1	B	348/404 (86%)	0.01	18 (5%) 31 35	36, 60, 130, 208	0
1	C	359/404 (88%)	-0.27	1 (0%) 94 95	33, 51, 85, 109	0
1	D	360/404 (89%)	-0.15	5 (1%) 78 80	27, 47, 92, 137	0
1	E	361/404 (89%)	-0.11	7 (1%) 70 73	36, 57, 97, 119	0
1	F	359/404 (88%)	-0.16	1 (0%) 94 95	36, 56, 91, 137	0
1	G	360/404 (89%)	-0.23	2 (0%) 90 91	35, 59, 93, 118	0
1	H	352/404 (87%)	0.58	46 (13%) 5 4	53, 96, 131, 194	0
All	All	2861/3232 (88%)	-0.07	84 (2%) 55 60	27, 57, 109, 208	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	1569	TYR	7.1
1	A	1789	GLU	6.1
1	B	1802	ILE	5.6
1	H	1835	ALA	5.5
1	F	1787	VAL	5.4
1	B	1799	ILE	5.2
1	H	1475	LEU	5.2
1	H	1518	ALA	5.0
1	H	1836	LEU	4.7
1	B	1758	THR	4.3
1	B	1798	PHE	4.3
1	B	1795	SER	4.3
1	H	1581	SER	4.2
1	H	1786	PRO	4.1
1	H	1520	TYR	4.0
1	H	1591	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	1578	HIS	3.7
1	H	1829	PHE	3.7
1	B	1756	LYS	3.3
1	D	1787	VAL	3.3
1	A	1471	PHE	3.2
1	E	1502	LEU	3.1
1	H	1848	GLY	3.1
1	D	1791	GLU	3.1
1	H	1588	LEU	3.1
1	H	1711	TRP	3.1
1	H	1834	LEU	3.1
1	H	1473	GLY	3.1
1	H	1839	ILE	3.1
1	D	1798	PHE	3.0
1	B	1786	PRO	3.0
1	B	1784	TYR	3.0
1	H	1586	HIS	3.0
1	H	1576	MET	2.8
1	H	1579	ASN	2.8
1	H	1850	ILE	2.8
1	H	1514	CYS	2.8
1	H	1785	THR	2.8
1	H	1853	VAL	2.8
1	H	1502	LEU	2.7
1	B	1783	LEU	2.7
1	H	1784	TYR	2.7
1	H	1849	PHE	2.7
1	B	1801	THR	2.7
1	H	1843	ALA	2.7
1	E	1793	ARG	2.6
1	H	1472	GLN	2.6
1	B	1806	LEU	2.6
1	D	1794	VAL	2.5
1	E	1479	ARG	2.5
1	H	1662	ILE	2.5
1	H	1852	ARG	2.4
1	H	1587	CYS	2.4
1	B	1807	ARG	2.4
1	G	1630	HIS	2.4
1	H	1804	MET	2.4
1	B	1766	CYS	2.4
1	E	1828	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	1471	PHE	2.3
1	D	1796	VAL	2.3
1	H	1847	LEU	2.3
1	H	1832	SER	2.3
1	H	1515	VAL	2.3
1	E	1804	MET	2.2
1	A	1790	PHE	2.2
1	H	1471	PHE	2.2
1	H	1513	MET	2.2
1	B	1800	ARG	2.2
1	H	1570	SER	2.1
1	H	1682	LEU	2.1
1	B	1502	LEU	2.1
1	H	1568	GLN	2.1
1	A	1794	VAL	2.1
1	C	1786	PRO	2.1
1	H	1669	PHE	2.1
1	H	1795	SER	2.1
1	E	1797	SER	2.1
1	E	1808	ASP	2.1
1	B	1780	VAL	2.1
1	H	1577	LYS	2.1
1	B	1797	SER	2.1
1	H	1521	LEU	2.0
1	H	1517	HIS	2.0
1	B	1765	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, 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	EDO	E	1902	4/4	0.91	0.28	17.46	59,61,65,70	0
2	EDO	A	1904	4/4	0.94	0.23	7.11	61,62,66,73	0
2	EDO	B	1902	4/4	0.97	0.22	6.45	64,65,66,67	0
2	EDO	D	1903	4/4	0.88	0.21	6.31	69,71,73,76	0
2	EDO	C	1902	4/4	0.98	0.17	3.80	41,43,45,51	0
2	EDO	G	1902	4/4	0.97	0.19	3.72	56,57,61,66	0
2	EDO	A	1902	4/4	0.95	0.17	3.58	49,50,51,52	0
2	EDO	H	1902	4/4	0.89	0.28	2.02	85,85,87,88	0
2	EDO	C	1903	4/4	0.94	0.16	1.74	48,50,55,63	0
2	EDO	E	1901	4/4	0.97	0.16	1.57	43,44,44,46	0
2	EDO	A	1903	4/4	0.92	0.23	1.19	55,55,57,60	0
2	EDO	H	1901	4/4	0.98	0.16	0.98	58,58,61,61	0
2	EDO	F	1902	4/4	0.97	0.13	0.74	54,56,58,58	0
2	EDO	B	1901	4/4	0.97	0.18	0.65	55,57,57,57	0
2	EDO	D	1901	4/4	0.98	0.19	0.50	39,43,46,47	0
2	EDO	F	1901	4/4	0.98	0.14	0.18	39,40,41,45	0
2	EDO	A	1901	4/4	0.98	0.17	0.16	36,36,37,38	0
2	EDO	D	1902	4/4	0.98	0.12	-0.05	42,45,45,46	0
2	EDO	G	1901	4/4	0.99	0.13	-0.07	35,36,36,40	0
2	EDO	F	1903	4/4	0.92	0.13	-0.33	53,56,56,60	0
2	EDO	C	1901	4/4	0.99	0.12	-0.65	36,43,48,49	0
2	EDO	G	1903	4/4	0.95	0.11	-1.59	56,59,67,73	0

6.5 Other polymers (i)

There are no such residues in this entry.