Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 07:23 PM EDT

PDB ID	:	4HPF
Title	:	Structure of the human SLO3 gating ring
Authors	:	Leonetti, M.D.; Yuan, P.; MacKinnon, R.
Deposited on	:	2012-10-23
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

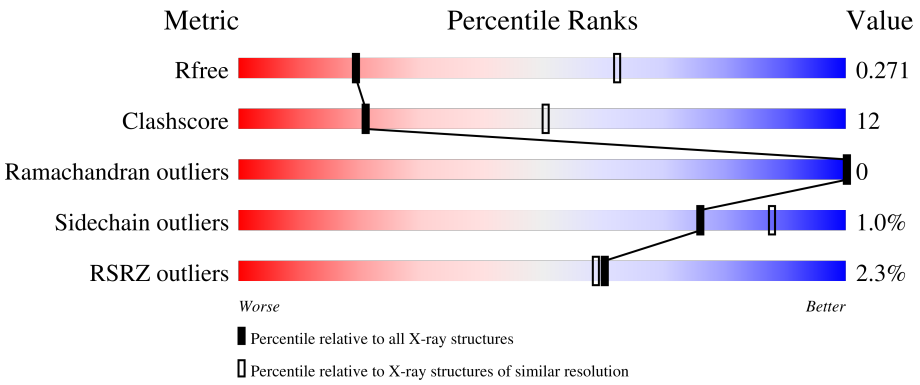
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	722	2% 60% 16% 24%
1	B	722	2% 59% 16% 25%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8241 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 Potassium channel subfamily U member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	4137	2666	694	748	29	0	0	0
1	B	543	4104	2646	687	742	29	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

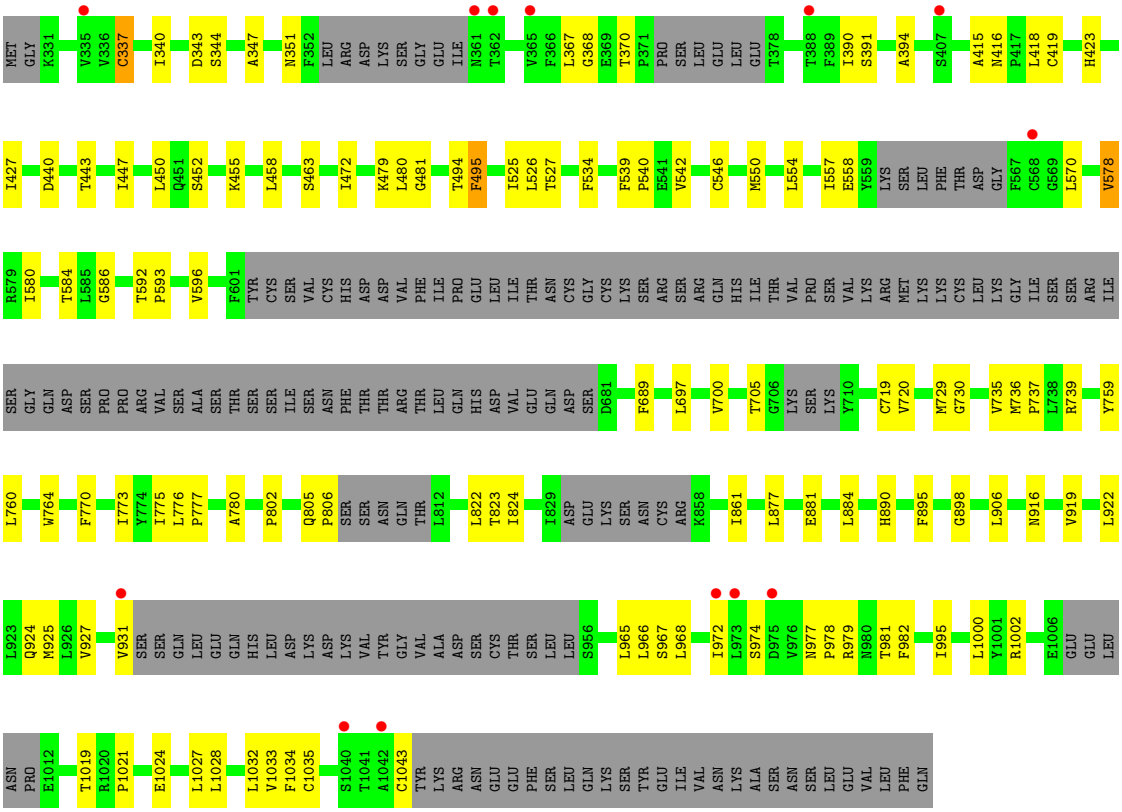
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	MET	-	initiating methionine	UNP A8MYU2
A	1063	SER	-	expression tag	UNP A8MYU2
A	1064	ASN	-	expression tag	UNP A8MYU2
A	1065	SER	-	expression tag	UNP A8MYU2
A	1066	LEU	-	expression tag	UNP A8MYU2
A	1067	GLU	-	expression tag	UNP A8MYU2
A	1068	VAL	-	expression tag	UNP A8MYU2
A	1069	LEU	-	expression tag	UNP A8MYU2
A	1070	PHE	-	expression tag	UNP A8MYU2
A	1071	GLN	-	expression tag	UNP A8MYU2
B	329	MET	-	initiating methionine	UNP A8MYU2
B	1063	SER	-	expression tag	UNP A8MYU2
B	1064	ASN	-	expression tag	UNP A8MYU2
B	1065	SER	-	expression tag	UNP A8MYU2
B	1066	LEU	-	expression tag	UNP A8MYU2
B	1067	GLU	-	expression tag	UNP A8MYU2
B	1068	VAL	-	expression tag	UNP A8MYU2
B	1069	LEU	-	expression tag	UNP A8MYU2
B	1070	PHE	-	expression tag	UNP A8MYU2
B	1071	GLN	-	expression tag	UNP A8MYU2

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

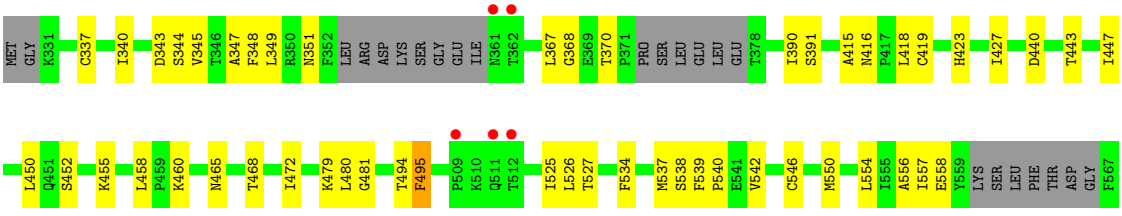
• Molecule 1: Potassium channel subfamily U member 1

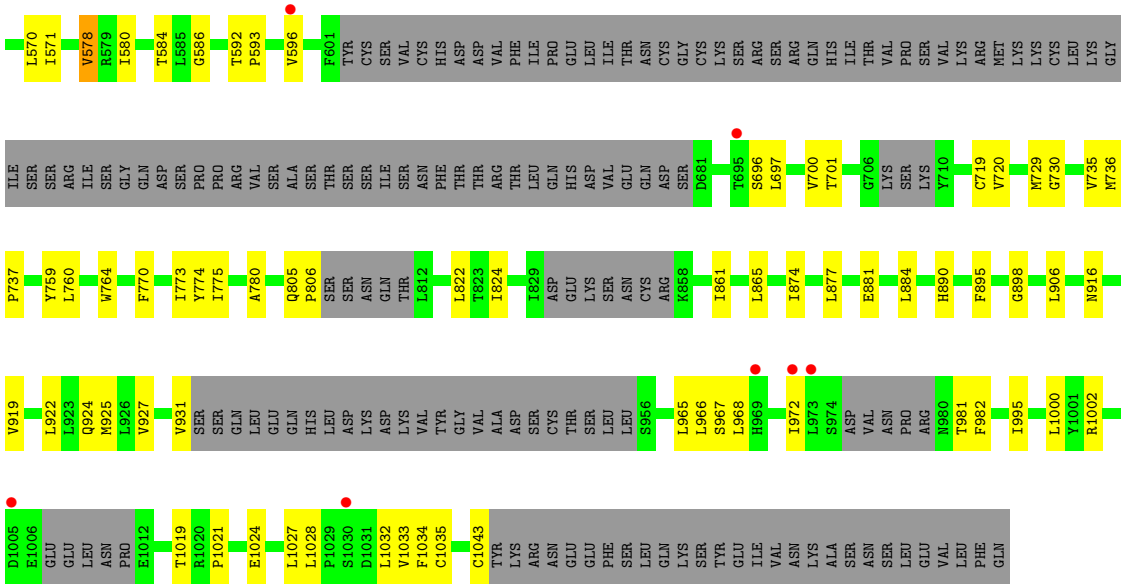
Chain A: 2% 60% 16% 24%



• Molecule 1: Potassium channel subfamily U member 1

Chain B: 2% 59% 16% 25%




L570 I571 V578 R579 I580 T584 L585 G586 T592 P593 V596 F601 TYR CYS SER VAL CYS HIS ASP ASP VAL PHE ILE PRO GLU LEU ILE THR ASN CYS GLY CYS LYS SER ARG SER ARG GLN HIS ILE THR VAL PRO SER VAL LYS ARG MET LYS LYS CYS LEU LYS GLY
ILE SER SER ARG ILE SER GLY GLN ASP SER PRO PRO ARG VAL SER ALA SER THR SER SER SER ILE SER ASN PHE THR THR ARG THR LEU GLN HIS ASP VAL GLU GLN ASP SER D681 T695 S696 L697 V700 T701 G706 LYS SER LYS Y710 C719 V720 M729 G730 V735 M736
P737 Y759 L760 W764 F770 I773 Y774 I775 A780 Q805 P806 SER SER ASN GLN THR L812 L822 T823 I824 I829 ASP GLU LYS SER ASN CYS ARG K858 I861 L865 I874 L877 E881 L884 H890 F895 G898 L906 N916
V919 L922 L923 Q924 M925 L926 V927 V931 SER SER GLN LEU GLU GLN HIS LEU ASP LYS ASP LYS VAL TYR GLY VAL ALA ASP SER CYS THR SER LEU LEU S956 L965 L966 S967 L968 H969 I972 L973 S974 ASP VAL ASN PRO ARG N980 T981 F982 I995 L1000 Y1001 R1002
D1005 E1006 GLU GLU LEU ASN PRO E1012 T1019 R1020 P1021 E1024 L1027 L1028 P1029 S1030 D1031 L1032 V1033 F1034 C1035 C1043 TYR LYS ARG ASN GLU GLU PHE SER LEU GLN LYS SER TYR GLU ILE VAL ASN LYS ALA SER ASN SER LEU GLU VAL LEU PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	124.54Å 157.94Å 249.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 3.40 48.49 – 3.32	Depositor EDS
% Data completeness (in resolution range)	89.9 (48.51-3.40) 84.4 (48.49-3.32)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.00 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.247 , 0.267 0.248 , 0.271	Depositor DCC
R_{free} test set	1583 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	65.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 34.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	8241	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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 (i)

5.1 Standard geometry (i)

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	0.48	0/4223	0.56	0/5741
1	B	0.48	0/4187	0.56	0/5688
All	All	0.48	0/8410	0.56	0/11429

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4137	0	3995	98	0
1	B	4104	0	3968	101	0
All	All	8241	0	7963	197	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 12.

All (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:SER:O	1:A:455:LYS:HG3	1.71	0.90
1:B:452:SER:O	1:B:455:LYS:HG3	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:LEU:HD11	1:A:775:ILE:HD12	1.58	0.85
1:A:966:LEU:HD12	1:A:1035:CYS:SG	2.20	0.82
1:B:697:LEU:HD11	1:B:775:ILE:HD12	1.61	0.81
1:B:966:LEU:HD12	1:B:1035:CYS:SG	2.23	0.79
1:A:458:LEU:HD13	1:A:472:ILE:HG21	1.68	0.76
1:B:495:PHE:CE1	1:B:1019:THR:HG22	2.21	0.75
1:B:458:LEU:HD13	1:B:472:ILE:HG21	1.68	0.74
1:B:447:ILE:HG23	1:B:472:ILE:HG22	1.70	0.73
1:A:447:ILE:HG23	1:A:472:ILE:HG22	1.70	0.72
1:A:916:ASN:ND2	1:A:919:VAL:HG23	2.05	0.71
1:A:447:ILE:CG2	1:A:472:ILE:HG22	2.22	0.70
1:B:344:SER:HA	1:B:347:ALA:HB3	1.74	0.69
1:B:495:PHE:CD1	1:B:1019:THR:HG22	2.28	0.69
1:A:977:ASN:CB	1:A:978:PRO:HD3	2.24	0.68
1:A:495:PHE:CE1	1:A:1019:THR:HG22	2.28	0.67
1:B:972:ILE:HG23	1:B:1043:CYS:C	2.15	0.67
1:A:340:ILE:CB	1:A:370:THR:OG1	2.42	0.67
1:A:494:THR:HG21	1:A:895:PHE:O	1.94	0.67
1:B:340:ILE:CB	1:B:370:THR:OG1	2.43	0.67
1:A:495:PHE:CD1	1:A:1019:THR:HG22	2.29	0.67
1:B:447:ILE:CG2	1:B:472:ILE:HG22	2.25	0.66
1:A:705:THR:HG21	1:B:696:SER:HB3	1.78	0.66
1:A:344:SER:HA	1:A:347:ALA:HB3	1.76	0.65
1:B:1002:ARG:HH12	1:B:1028:LEU:HD13	1.62	0.65
1:A:1002:ARG:HH12	1:A:1028:LEU:HD13	1.61	0.64
1:A:720:VAL:HG21	1:A:760:LEU:HD21	1.81	0.63
1:A:347:ALA:O	1:A:351:ASN:ND2	2.23	0.63
1:B:494:THR:HG21	1:B:895:PHE:O	1.99	0.62
1:B:700:VAL:HG13	1:B:773:ILE:O	1.99	0.62
1:B:720:VAL:HG21	1:B:760:LEU:HD21	1.81	0.61
1:A:968:LEU:HD22	1:A:979:ARG:HD2	1.81	0.61
1:B:525:ILE:HD13	1:B:922:LEU:CD2	2.31	0.61
1:B:527:THR:HG21	1:B:916:ASN:HD21	1.64	0.60
1:B:916:ASN:ND2	1:B:919:VAL:HG23	2.16	0.60
1:A:700:VAL:HG13	1:A:773:ILE:O	2.01	0.60
1:B:924:GLN:HG2	1:B:931:VAL:HG22	1.84	0.60
1:A:924:GLN:HG2	1:A:931:VAL:HG22	1.84	0.59
1:A:525:ILE:HD13	1:A:922:LEU:HD23	1.84	0.58
1:B:525:ILE:HD13	1:B:922:LEU:HD23	1.83	0.58
1:B:534:PHE:CE1	1:B:542:VAL:HG13	2.38	0.58
1:A:539:PHE:CE1	1:A:554:LEU:HD21	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:LEU:HD13	1:A:877:LEU:HD22	1.85	0.57
1:A:525:ILE:HD13	1:A:922:LEU:CD2	2.35	0.57
1:B:481:GLY:HA3	1:B:927:VAL:CG1	2.35	0.57
1:B:481:GLY:HA3	1:B:927:VAL:HG13	1.86	0.57
1:B:479:LYS:HG2	1:B:906:LEU:HD12	1.86	0.56
1:B:539:PHE:CE1	1:B:554:LEU:HD21	2.40	0.56
1:A:481:GLY:HA3	1:A:927:VAL:CG1	2.35	0.56
1:A:534:PHE:CE1	1:A:542:VAL:HG13	2.41	0.56
1:A:481:GLY:HA3	1:A:927:VAL:HG13	1.86	0.56
1:A:455:LYS:HB3	1:A:472:ILE:HD12	1.87	0.55
1:A:479:LYS:HG2	1:A:906:LEU:HD12	1.88	0.55
1:A:982:PHE:HA	1:A:1027:LEU:HD11	1.89	0.54
1:A:494:THR:HG21	1:A:898:GLY:HA2	1.90	0.54
1:B:415:ALA:HB1	1:B:450:LEU:HD13	1.89	0.54
1:B:822:LEU:HD13	1:B:877:LEU:HD22	1.89	0.54
1:B:423:HIS:HD2	1:B:427:ILE:HD13	1.73	0.54
1:B:455:LYS:HB3	1:B:472:ILE:HD12	1.89	0.54
1:A:458:LEU:HD13	1:A:472:ILE:CG2	2.37	0.53
1:A:343:ASP:OD1	1:A:347:ALA:HB2	2.09	0.53
1:B:534:PHE:CD1	1:B:542:VAL:HG13	2.43	0.53
1:B:570:LEU:CD2	1:B:925:MET:SD	2.96	0.53
1:A:480:LEU:HD12	1:A:730:GLY:O	2.08	0.53
1:B:697:LEU:CD1	1:B:775:ILE:HD12	2.36	0.52
1:B:458:LEU:HD13	1:B:472:ILE:CG2	2.38	0.52
1:B:495:PHE:CD1	1:B:1019:THR:CG2	2.92	0.52
1:B:343:ASP:OD1	1:B:347:ALA:HB2	2.09	0.52
1:B:494:THR:HG21	1:B:898:GLY:HA2	1.91	0.52
1:A:697:LEU:CD1	1:A:775:ILE:HD12	2.34	0.52
1:B:347:ALA:O	1:B:351:ASN:ND2	2.30	0.51
1:B:729:MET:HG2	1:B:759:TYR:OH	2.10	0.51
1:A:972:ILE:HG23	1:A:1043:CYS:C	2.31	0.51
1:A:495:PHE:CD1	1:A:495:PHE:C	2.84	0.51
1:A:534:PHE:CD1	1:A:542:VAL:HG13	2.46	0.51
1:B:982:PHE:HA	1:B:1027:LEU:HD11	1.93	0.51
1:B:1024:GLU:O	1:B:1024:GLU:HG2	2.11	0.51
1:A:415:ALA:HB1	1:A:450:LEU:HD13	1.93	0.50
1:B:416:ASN:OD1	1:B:418:LEU:HA	2.11	0.50
1:B:527:THR:HG21	1:B:916:ASN:ND2	2.26	0.50
1:B:416:ASN:HB2	1:B:450:LEU:HD11	1.94	0.50
1:B:805:GLN:HB3	1:B:806:PRO:HD2	1.94	0.50
1:B:495:PHE:CD1	1:B:495:PHE:C	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:LEU:HD23	1:B:368:GLY:N	2.27	0.49
1:A:416:ASN:OD1	1:A:418:LEU:HA	2.11	0.49
1:A:539:PHE:HB3	1:A:540:PRO:HD3	1.95	0.49
1:A:824:ILE:HG21	1:A:861:ILE:HD12	1.94	0.49
1:A:1024:GLU:HG2	1:A:1024:GLU:O	2.12	0.49
1:B:1000:LEU:CD2	1:B:1033:VAL:HG22	2.43	0.49
1:B:578:VAL:HG22	1:B:578:VAL:O	2.10	0.49
1:A:965:LEU:HD13	1:A:1034:PHE:CE1	2.47	0.49
1:A:805:GLN:HB3	1:A:806:PRO:HD2	1.94	0.49
1:B:557:ILE:HG22	1:B:586:GLY:HA2	1.95	0.48
1:A:770:PHE:HB2	1:A:773:ILE:HD12	1.95	0.48
1:B:539:PHE:HB3	1:B:540:PRO:HD3	1.95	0.48
1:A:494:THR:CG2	1:A:898:GLY:HA2	2.44	0.48
1:A:570:LEU:CD2	1:A:925:MET:SD	3.02	0.48
1:A:965:LEU:HD13	1:A:1034:PHE:CD1	2.49	0.48
1:A:974:SER:O	1:A:979:ARG:NH1	2.47	0.48
1:B:981:THR:OG1	1:B:1024:GLU:HA	2.14	0.48
1:A:557:ILE:HG22	1:A:586:GLY:HA2	1.95	0.48
1:B:527:THR:CG2	1:B:916:ASN:HD21	2.27	0.48
1:B:824:ILE:HG21	1:B:861:ILE:HD12	1.95	0.48
1:A:423:HIS:HD2	1:A:427:ILE:HD13	1.79	0.48
1:B:480:LEU:HD12	1:B:730:GLY:O	2.14	0.48
1:A:1000:LEU:CD2	1:A:1033:VAL:HG22	2.44	0.47
1:A:527:THR:HG21	1:A:916:ASN:HD21	1.79	0.47
1:B:525:ILE:HG22	1:B:525:ILE:O	2.13	0.47
1:A:367:LEU:HD23	1:A:368:GLY:N	2.29	0.47
1:A:982:PHE:CG	1:A:1021:PRO:HG2	2.50	0.47
1:A:416:ASN:HB2	1:A:450:LEU:HD11	1.97	0.47
1:A:719:CYS:HB3	1:A:780:ALA:HB2	1.97	0.47
1:A:982:PHE:HB2	1:A:1027:LEU:HD21	1.97	0.47
1:A:1002:ARG:HH11	1:A:1028:LEU:HD22	1.78	0.47
1:A:415:ALA:CB	1:A:450:LEU:HD13	2.45	0.47
1:A:495:PHE:CD1	1:A:1019:THR:CG2	2.98	0.47
1:A:558:GLU:O	1:A:584:THR:HG23	2.15	0.46
1:B:982:PHE:CG	1:B:1021:PRO:HG2	2.50	0.46
1:B:1002:ARG:NH1	1:B:1028:LEU:HD13	2.30	0.46
1:A:972:ILE:HD11	1:A:995:ILE:HD12	1.97	0.46
1:A:981:THR:OG1	1:A:1024:GLU:HA	2.15	0.46
1:A:729:MET:HG2	1:A:759:TYR:OH	2.15	0.46
1:A:735:VAL:HG11	1:A:773:ILE:HD11	1.98	0.46
1:B:415:ALA:CB	1:B:450:LEU:HD13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:VAL:CG1	1:A:773:ILE:O	2.64	0.46
1:A:337:CYS:SG	1:A:394:ALA:HB2	2.56	0.45
1:B:967:SER:HA	1:B:1032:LEU:CD2	2.46	0.45
1:B:546:CYS:HA	1:B:550:MET:CE	2.47	0.45
1:B:539:PHE:HE1	1:B:554:LEU:HD21	1.82	0.45
1:B:494:THR:CG2	1:B:898:GLY:HA2	2.46	0.45
1:B:423:HIS:CD2	1:B:427:ILE:HD13	2.51	0.45
1:B:1002:ARG:HH11	1:B:1028:LEU:HD22	1.81	0.45
1:A:495:PHE:C	1:A:495:PHE:HD1	2.20	0.45
1:B:700:VAL:CG1	1:B:773:ILE:O	2.63	0.45
1:B:967:SER:O	1:B:968:LEU:HB2	2.16	0.45
1:B:972:ILE:HD11	1:B:995:ILE:HD12	1.97	0.45
1:A:526:LEU:HD22	1:A:593:PRO:HB3	1.99	0.45
1:B:539:PHE:CE1	1:B:554:LEU:CD2	3.00	0.45
1:A:440:ASP:OD2	1:A:443:THR:HG23	2.17	0.44
1:A:526:LEU:HB2	1:A:596:VAL:HG21	1.99	0.44
1:A:539:PHE:CE1	1:A:554:LEU:CD2	3.00	0.44
1:B:1024:GLU:OE1	1:B:1024:GLU:N	2.47	0.44
1:B:735:VAL:HG11	1:B:773:ILE:HD11	1.99	0.44
1:A:967:SER:O	1:A:968:LEU:HB2	2.18	0.44
1:A:423:HIS:CD2	1:A:427:ILE:HD13	2.53	0.44
1:A:1002:ARG:NH1	1:A:1028:LEU:HD13	2.28	0.44
1:B:558:GLU:O	1:B:584:THR:HG23	2.18	0.44
1:A:480:LEU:CD1	1:A:730:GLY:O	2.66	0.44
1:A:689:PHE:HB2	1:A:739:ARG:O	2.18	0.44
1:B:697:LEU:O	1:B:701:THR:HG22	2.17	0.44
1:A:525:ILE:O	1:A:525:ILE:HG22	2.17	0.44
1:A:736:MET:HB3	1:A:737:PRO:HD3	1.99	0.43
1:A:390:ILE:HG22	1:A:391:SER:N	2.34	0.43
1:B:526:LEU:HD22	1:B:593:PRO:HB3	2.00	0.43
1:B:390:ILE:HG22	1:B:391:SER:N	2.33	0.43
1:A:776:LEU:HD12	1:A:777:PRO:HD2	2.01	0.43
1:B:526:LEU:HB2	1:B:596:VAL:HG21	2.01	0.43
1:B:719:CYS:HB3	1:B:780:ALA:HB2	1.99	0.43
1:B:556:ALA:HB1	1:B:571:ILE:O	2.18	0.43
1:B:770:PHE:HB2	1:B:773:ILE:HD12	1.99	0.43
1:B:965:LEU:HD13	1:B:1034:PHE:CD1	2.54	0.43
1:A:967:SER:HA	1:A:1032:LEU:CD2	2.49	0.43
1:A:539:PHE:HE1	1:A:554:LEU:HD21	1.81	0.42
1:A:578:VAL:O	1:A:578:VAL:HG22	2.19	0.42
1:B:982:PHE:HB2	1:B:1027:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:THR:HG22	1:B:460:LYS:NZ	2.34	0.42
1:A:977:ASN:CB	1:A:978:PRO:CD	2.96	0.42
1:A:1024:GLU:OE1	1:A:1024:GLU:N	2.47	0.42
1:B:344:SER:O	1:B:348:PHE:N	2.51	0.42
1:B:965:LEU:HD13	1:B:1034:PHE:CE1	2.54	0.42
1:A:592:THR:HB	1:A:593:PRO:HD2	2.02	0.42
1:B:890:HIS:HA	1:B:895:PHE:CD2	2.54	0.42
1:B:390:ILE:CG2	1:B:391:SER:N	2.82	0.42
1:B:423:HIS:CD2	1:B:427:ILE:CD1	3.03	0.42
1:B:495:PHE:C	1:B:495:PHE:HD1	2.22	0.42
1:B:865:LEU:HD11	1:B:874:ILE:HD11	2.01	0.42
1:A:390:ILE:CG2	1:A:391:SER:N	2.83	0.41
1:B:345:VAL:O	1:B:349:LEU:CB	2.67	0.41
1:B:440:ASP:OD2	1:B:443:THR:HG23	2.20	0.41
1:B:465:ASN:OD1	1:B:468:THR:HG23	2.20	0.41
1:B:538:SER:O	1:B:542:VAL:HG23	2.19	0.41
1:B:700:VAL:HG21	1:B:764:TRP:CZ2	2.55	0.41
1:A:700:VAL:HG21	1:A:764:TRP:CZ2	2.55	0.41
1:B:537:MET:HB3	1:B:537:MET:HE2	1.98	0.41
1:A:890:HIS:HA	1:A:895:PHE:CD2	2.55	0.41
1:B:700:VAL:CG1	1:B:774:TYR:HA	2.51	0.41
1:B:736:MET:HB3	1:B:737:PRO:HD3	2.01	0.41
1:B:881:GLU:OE2	1:B:884:LEU:HD12	2.20	0.41
1:A:539:PHE:HA	1:A:580:ILE:HD11	2.03	0.41
1:A:881:GLU:OE2	1:A:884:LEU:HD12	2.21	0.41
1:B:592:THR:HB	1:B:593:PRO:HD2	2.02	0.41
1:A:546:CYS:HA	1:A:550:MET:CE	2.51	0.41
1:A:966:LEU:CD1	1:A:1035:CYS:SG	3.01	0.41
1:A:729:MET:CE	1:A:802:PRO:HA	2.52	0.40
1:B:700:VAL:HG12	1:B:774:TYR:HA	2.04	0.40
1:B:539:PHE:HA	1:B:580:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	528/722 (73%)	496 (94%)	32 (6%)	0	100	100
1	B	521/722 (72%)	491 (94%)	30 (6%)	0	100	100
All	All	1049/1444 (73%)	987 (94%)	62 (6%)	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	435/650 (67%)	430 (99%)	5 (1%)	73	86
1	B	431/650 (66%)	427 (99%)	4 (1%)	78	90
All	All	866/1300 (67%)	857 (99%)	9 (1%)	76	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	CYS
1	A	419	CYS
1	A	463	SER
1	A	495	PHE
1	A	578	VAL
1	B	337	CYS
1	B	419	CYS
1	B	495	PHE
1	B	578	VAL

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

Mol	Chain	Res	Type
1	A	423	HIS

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Mol	Chain	Res	Type
1	A	885	GLN
1	A	916	ASN
1	B	423	HIS
1	B	451	GLN
1	B	916	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	548/722 (75%)	-0.01	13 (2%)	59	57	31, 65, 110, 140	0
1	B	543/722 (75%)	-0.02	12 (2%)	62	60	30, 65, 110, 123	0
All	All	1091/1444 (75%)	-0.02	25 (2%)	60	59	30, 65, 110, 140	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	ASN	3.4
1	B	362	THR	3.3
1	A	362	THR	3.1
1	B	512	THR	2.9
1	A	1040	SER	2.7
1	A	568	CYS	2.7
1	B	973	LEU	2.6
1	B	509	PRO	2.6
1	B	511	GLN	2.6
1	A	407	SER	2.5
1	B	1030	SER	2.4
1	B	695	THR	2.4
1	A	365	VAL	2.4
1	A	975	ASP	2.3
1	B	1005	ASP	2.3
1	A	972	ILE	2.3
1	A	335	VAL	2.2
1	A	361	ASN	2.2
1	B	969	HIS	2.2
1	A	973	LEU	2.1
1	A	931	VAL	2.1
1	B	972	ILE	2.1
1	A	388	THR	2.1
1	B	596	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1042	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.