Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:37 PM GMT

PDB ID	:	1L5J
Title	:	CRYSTAL STRUCTURE OF E. COLI ACONITASE B.
Authors	:	Williams, C.H.; Stillman, T.J.; Barynin, V.V.; Sedelnikova, S.E.; Tang, Y.; Green, J.; Guest, J.R.; Artymiuk, P.J.
Deposited on	:	2002-03-07
Resolution	:	2.40 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
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:

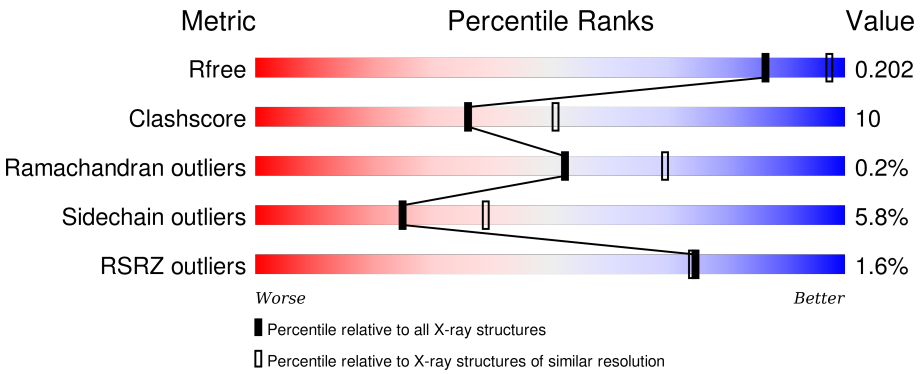
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	865	2% 79% 18% •
1	B	865	% 79% 18% •

2 Entry composition (i)

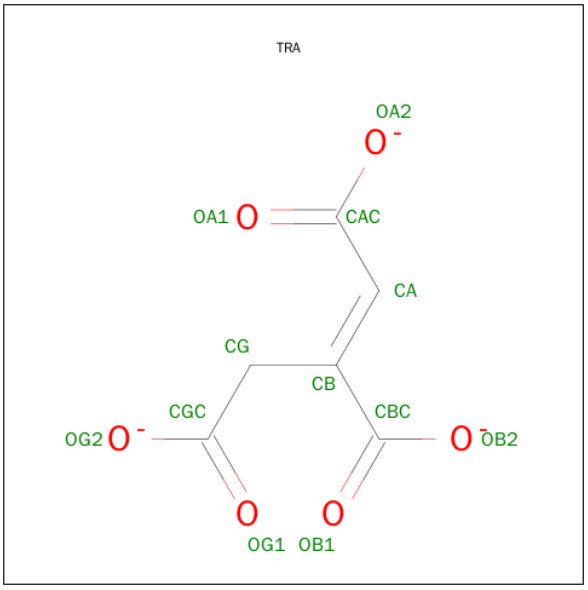
There are 4 unique types of molecules in this entry. The entry contains 13712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aconitate hydratase 2.

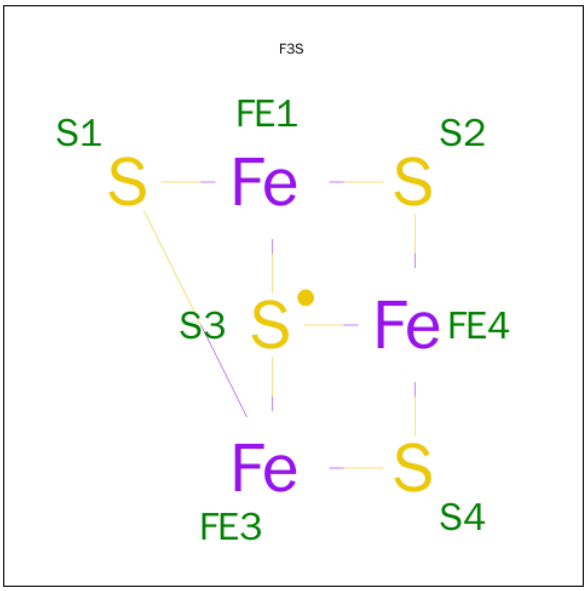
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	862	6552	4152	1122	1245	33	0	0	0
1	B	862	6552	4152	1122	1245	33	0	0	0

- Molecule 2 is ACONITATE ION (three-letter code: TRA) (formula: $C_6H_3O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0
2	B	1	12	6	6	0	0

- Molecule 3 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	7	3	4	0	0
			Total	Fe	S		
3	B	1	7	3	4	0	0

- Molecule 4 is water.

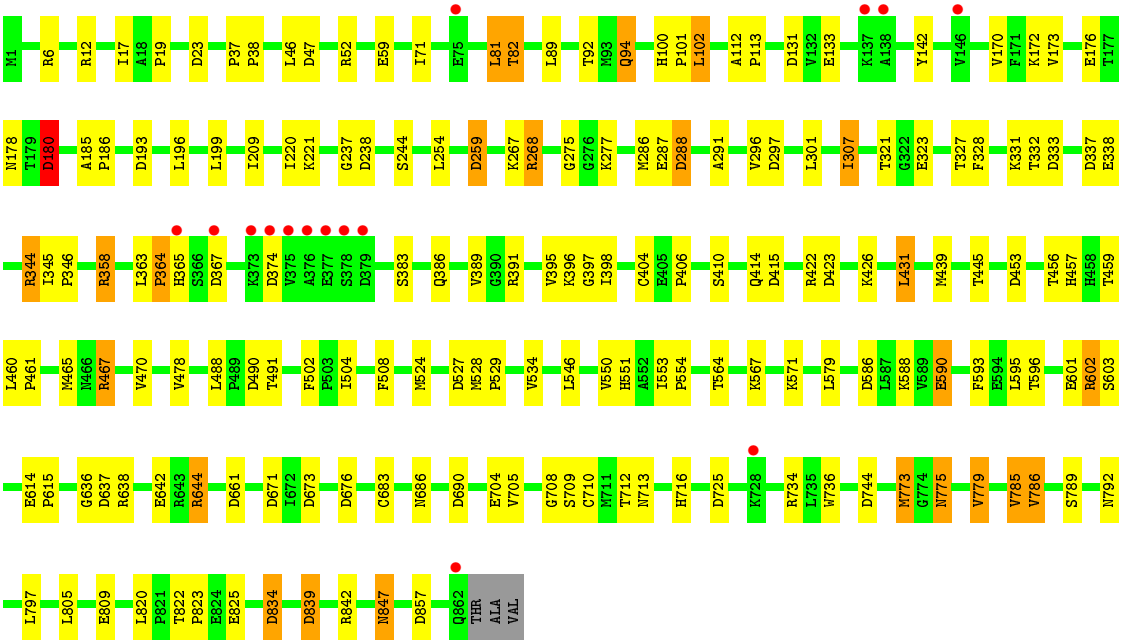
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	294	294	294	0	0
			Total	O		
4	B	276	276	276	0	0

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.

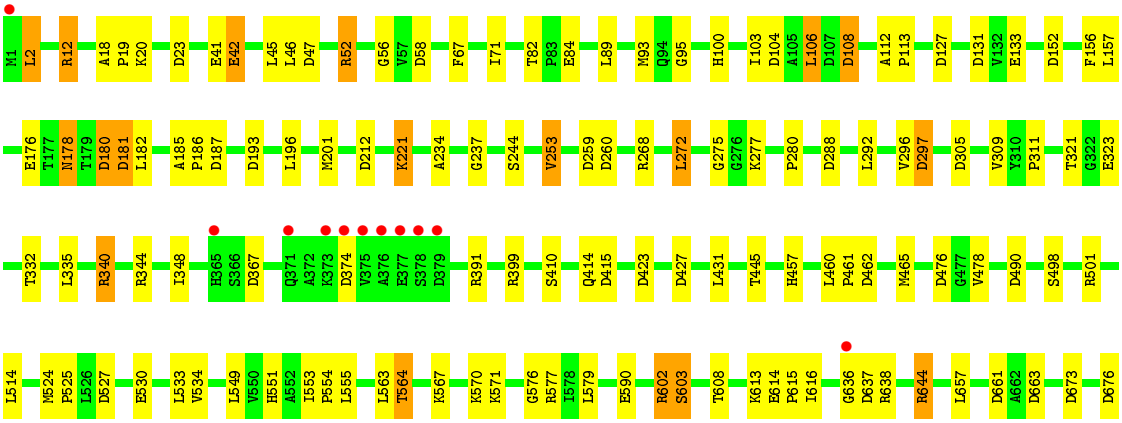
- Molecule 1: Aconitate hydratase 2

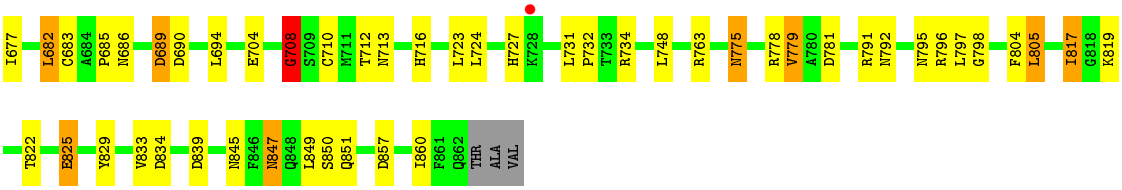
Chain A:



- Molecule 1: Aconitate hydratase 2

Chain B:




I677
L682
C683
A684
F685
N686
D689
D690
L694
E704
G708
S709
C710
N711
T712
N713
H716
L723
L724
H727
K728
L731
P732
T733
R734
L748
R763
N775
R778
V779
A780
D781
R791
N792
N795
R796
L797
G798
F804
L805
I817
G818
K819
T822
E825
Y829
V833
D834
D839
N845
F846
N847
Q848
L849
S850
Q851
D857
I860
F861
Q862
THR
ALA
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	138.97Å 169.63Å 113.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.10 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.40) 96.0 (20.10-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.151 , 0.203 0.155 , 0.202	Depositor DCC
R_{free} test set	5019 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 100794 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13712	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TRA, F3S

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	0.34	0/6686	0.75	26/9076 (0.3%)
1	B	0.35	0/6686	0.77	36/9076 (0.4%)
All	All	0.35	0/13372	0.76	62/18152 (0.3%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	288	ASP	CB-CG-OD2	6.52	124.16	118.30
1	B	637	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	104	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	676	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	476	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	297	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	744	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	527	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	181	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	23	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	663	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	131	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	333	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	423	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	673	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	857	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	527	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	288	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	690	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	423	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	637	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	708	GLY	N-CA-C	5.49	126.83	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	781	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	127	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	131	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	839	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	725	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	23	ASP	CB-CA-C	-5.43	99.53	110.40
1	B	305	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	462	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	180	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	108	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	259	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	857	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	676	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	839	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	427	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	47	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	689	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	834	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	490	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	367	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	690	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	238	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	260	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	47	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	180	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	374	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	367	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	337	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	490	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	297	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	661	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	58	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	671	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	661	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	834	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	187	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	586	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	152	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	374	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	673	ASP	CB-CG-OD2	5.02	122.82	118.30

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	6552	0	6569	129	0
1	B	6552	0	6569	122	0
2	A	12	0	3	2	0
2	B	12	0	3	2	0
3	A	7	0	0	0	0
3	B	7	0	0	0	0
4	A	294	0	0	15	0
4	B	276	0	0	11	0
All	All	13712	0	13144	251	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 10.

All (251) 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:B:530:GLU:OE2	1:B:577:ARG:NH1	1.79	1.15
1:A:439:MET:HE2	4:A:1105:HOH:O	1.56	1.06
1:B:465:MET:SD	1:B:636:GLY:HA3	1.98	1.03
1:B:178:ASN:ND2	1:B:180:ASP:H	1.55	1.03
1:A:439:MET:HB3	4:A:1105:HOH:O	1.60	1.00
1:A:321:THR:CG2	1:A:323:GLU:HG3	1.91	0.99
1:A:301:LEU:HD22	1:A:307:ILE:HD11	1.45	0.99
1:A:296:VAL:HG12	1:A:328:PHE:HB3	1.44	0.98
1:B:590:GLU:HG3	4:B:931:HOH:O	1.64	0.97
1:B:686:ASN:HA	1:B:792:ASN:O	1.65	0.96
1:B:178:ASN:HD22	1:B:180:ASP:H	1.13	0.96
1:B:847:ASN:HD22	1:B:847:ASN:H	1.13	0.96
1:A:590:GLU:HG2	4:A:888:HOH:O	1.66	0.95
1:A:564:THR:HG22	1:A:571:LYS:H	1.30	0.94
1:B:708:GLY:O	4:B:1117:HOH:O	1.87	0.93
1:A:296:VAL:CG1	1:A:328:PHE:HB3	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ASN:HA	1:A:792:ASN:O	1.70	0.90
1:A:847:ASN:HD22	1:A:847:ASN:H	1.19	0.89
1:A:321:THR:HG22	1:A:323:GLU:HG3	1.55	0.88
1:A:286:MET:HG3	1:A:291:ALA:HB3	1.53	0.88
1:A:775:ASN:HD22	1:A:775:ASN:H	1.23	0.87
1:B:52:ARG:HD3	4:B:878:HOH:O	1.72	0.87
1:A:301:LEU:HD22	1:A:307:ILE:CD1	2.08	0.83
1:B:778:ARG:CZ	4:B:1052:HOH:O	2.25	0.83
1:B:410:SER:OG	1:B:644:ARG:NH2	2.12	0.83
1:A:89:LEU:O	1:A:92:THR:HG22	1.80	0.82
1:B:478:VAL:HG11	1:B:710:CYS:HB3	1.63	0.81
1:A:52:ARG:HD3	4:A:957:HOH:O	1.80	0.80
1:A:331:LYS:HG3	1:A:332:THR:HG23	1.62	0.80
1:A:564:THR:CG2	1:A:571:LYS:H	1.95	0.80
1:A:288:ASP:OD1	1:A:344:ARG:HD2	1.80	0.80
1:B:178:ASN:HD22	1:B:180:ASP:N	1.79	0.79
1:B:775:ASN:HD22	1:B:775:ASN:H	1.30	0.79
1:B:465:MET:SD	1:B:636:GLY:CA	2.73	0.77
1:B:100:HIS:HB3	4:B:1130:HOH:O	1.84	0.77
1:A:321:THR:HG21	1:A:323:GLU:HG3	1.67	0.75
1:A:488:LEU:O	1:A:491:THR:HG22	1.85	0.75
1:A:773:MET:HG2	1:A:775:ASN:ND2	2.02	0.75
1:B:817:ILE:HG22	1:B:819:LYS:HG2	1.69	0.74
1:A:259:ASP:O	1:A:268:ARG:HG3	1.86	0.74
1:A:267:LYS:HE2	4:A:1090:HOH:O	1.87	0.74
1:A:713:ASN:H	1:A:716:HIS:CD2	2.08	0.72
1:A:12:ARG:NH2	1:A:193:ASP:OD2	2.18	0.72
1:A:358:ARG:HH11	1:A:358:ARG:HG2	1.53	0.71
1:B:259:ASP:O	1:B:268:ARG:HG3	1.89	0.71
1:A:713:ASN:H	1:A:716:HIS:HD2	1.38	0.71
1:A:410:SER:OG	1:A:644:ARG:NH2	2.23	0.71
1:B:554:PRO:HG3	1:B:602:ARG:CZ	2.22	0.70
1:A:465:MET:SD	1:A:636:GLY:HA2	2.31	0.70
1:B:822:THR:H	1:B:825:GLU:HG3	1.57	0.70
1:B:817:ILE:CG2	1:B:819:LYS:HG2	2.23	0.69
1:B:415:ASP:OD2	1:B:445:THR:HG22	1.93	0.69
1:A:71:ILE:HG21	1:A:81:LEU:HD13	1.73	0.68
1:B:178:ASN:ND2	1:B:180:ASP:N	2.37	0.67
1:A:636:GLY:N	4:A:905:HOH:O	2.22	0.67
1:B:234:ALA:HB1	1:B:272:LEU:CD1	2.24	0.67
1:B:704:GLU:CD	1:B:779:VAL:HG22	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:HG22	1:A:209:ILE:HD11	1.77	0.66
1:A:704:GLU:CD	1:A:779:VAL:HG22	2.16	0.66
1:A:590:GLU:CG	4:A:888:HOH:O	2.35	0.65
1:B:234:ALA:HB2	1:B:272:LEU:HD11	1.78	0.65
1:B:201:MET:HE1	1:B:253:VAL:HB	1.79	0.65
1:B:280:PRO:HG3	1:B:576:GLY:HA2	1.79	0.65
1:A:259:ASP:C	1:A:268:ARG:HG3	2.16	0.65
1:B:234:ALA:CB	1:B:272:LEU:HD11	2.27	0.64
1:B:182:LEU:HD22	1:B:201:MET:HE2	1.78	0.64
1:A:638:ARG:HD3	1:A:642:GLU:OE1	1.97	0.63
1:B:234:ALA:CB	1:B:272:LEU:CD1	2.76	0.63
1:B:833:VAL:HG12	1:B:833:VAL:O	1.99	0.62
1:B:713:ASN:H	1:B:716:HIS:HD2	1.46	0.61
1:A:847:ASN:HD22	1:A:847:ASN:N	1.95	0.61
1:B:321:THR:HG21	1:B:323:GLU:HG3	1.83	0.60
1:B:514:LEU:HD11	1:B:525:PRO:HD2	1.82	0.60
1:B:683:CYS:HB2	1:B:805:LEU:HB2	1.82	0.60
1:A:775:ASN:N	1:A:775:ASN:HD22	1.94	0.60
1:B:445:THR:HG23	1:B:457:HIS:NE2	2.17	0.60
1:A:244:SER:HB2	2:A:866:TRA:OG1	2.02	0.60
1:B:713:ASN:H	1:B:716:HIS:CD2	2.20	0.60
1:B:847:ASN:ND2	1:B:847:ASN:H	1.92	0.60
1:B:685:PRO:HD3	1:B:804:PHE:CE2	2.36	0.60
1:B:847:ASN:N	1:B:847:ASN:HD22	1.92	0.59
1:A:383:SER:H	1:A:386:GLN:NE2	2.01	0.59
1:A:296:VAL:CG1	1:A:328:PHE:CB	2.78	0.59
1:A:847:ASN:ND2	1:A:847:ASN:H	1.97	0.59
1:A:395:VAL:HG12	1:A:397:GLY:H	1.68	0.59
1:A:406:PRO:HD2	1:A:524:MET:O	2.02	0.59
1:A:478:VAL:HG11	1:A:710:CYS:HB3	1.85	0.58
1:A:593:PHE:HA	1:A:596:THR:HG22	1.84	0.58
1:B:833:VAL:CG1	1:B:833:VAL:O	2.51	0.58
1:B:67:PHE:CZ	1:B:71:ILE:HD11	2.39	0.58
1:B:778:ARG:NE	4:B:1052:HOH:O	2.34	0.58
1:A:459:THR:HG23	4:A:971:HOH:O	2.02	0.58
1:B:822:THR:OG1	1:B:825:GLU:HG2	2.05	0.57
1:A:395:VAL:HG12	1:A:396:LYS:N	2.18	0.57
1:B:614:GLU:HB2	1:B:615:PRO:HD3	1.86	0.57
1:A:185:ALA:HB3	1:A:186:PRO:HD3	1.86	0.57
1:B:259:ASP:C	1:B:268:ARG:HG3	2.25	0.56
1:B:20:LYS:HE2	1:B:193:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:THR:HG21	1:A:323:GLU:CG	2.34	0.56
1:A:112:ALA:HB3	1:A:113:PRO:HD3	1.87	0.56
1:A:237:GLY:O	1:A:275:GLY:HA2	2.05	0.56
1:B:182:LEU:HD22	1:B:201:MET:CE	2.35	0.56
1:A:554:PRO:HG3	1:A:602:ARG:CZ	2.37	0.55
1:A:358:ARG:HH11	1:A:358:ARG:CG	2.20	0.55
1:A:602:ARG:O	1:A:603:SER:HB2	2.06	0.55
1:B:704:GLU:HG2	1:B:734:ARG:HB3	1.87	0.55
1:B:553:ILE:HB	1:B:554:PRO:HD3	1.89	0.54
1:B:682:LEU:N	1:B:682:LEU:HD23	2.22	0.54
1:A:170:VAL:HG21	1:A:307:ILE:HD12	1.89	0.54
1:A:389:VAL:HG12	1:A:398:ILE:HD12	1.88	0.54
1:B:12:ARG:HD2	1:B:19:PRO:HA	1.90	0.54
1:A:712:THR:HA	1:A:716:HIS:CD2	2.43	0.54
1:A:12:ARG:HD3	1:A:17:ILE:HG13	1.89	0.54
1:B:817:ILE:HD11	1:B:829:TYR:OH	2.07	0.54
1:B:704:GLU:OE2	1:B:779:VAL:HG22	2.08	0.53
1:A:773:MET:O	1:A:773:MET:HG3	2.08	0.53
1:B:613:LYS:HD3	4:B:961:HOH:O	2.09	0.53
1:A:395:VAL:CG1	1:A:396:LYS:N	2.72	0.53
1:B:344:ARG:O	1:B:348:ILE:HG12	2.08	0.53
1:B:685:PRO:HD3	1:B:804:PHE:CD2	2.44	0.53
1:A:100:HIS:HB2	1:A:101:PRO:HD3	1.90	0.53
1:B:112:ALA:HB3	1:B:113:PRO:HD3	1.91	0.53
1:A:705:VAL:HG22	1:A:786:VAL:CG1	2.39	0.52
1:A:465:MET:SD	1:A:636:GLY:CA	2.96	0.52
1:A:553:ILE:HB	1:A:554:PRO:HD3	1.91	0.52
1:B:212:ASP:OD1	1:B:221:LYS:HD3	2.10	0.52
1:A:705:VAL:HG22	1:A:786:VAL:HG13	1.92	0.52
1:A:358:ARG:HG3	1:A:363:LEU:HB2	1.92	0.52
1:A:683:CYS:HB2	1:A:805:LEU:HB2	1.93	0.51
1:A:92:THR:HG21	4:A:877:HOH:O	2.11	0.51
1:B:551:HIS:O	1:B:554:PRO:HD2	2.10	0.51
1:A:199:LEU:HD22	1:A:220:ILE:CD1	2.40	0.51
1:A:422:ARG:HD3	1:A:426:LYS:HE2	1.92	0.51
1:A:345:ILE:HB	1:A:346:PRO:HD3	1.93	0.51
1:B:792:ASN:HB3	1:B:805:LEU:HD13	1.93	0.50
1:B:445:THR:CG2	1:B:457:HIS:NE2	2.74	0.50
1:A:286:MET:HG3	1:A:291:ALA:CB	2.35	0.50
1:B:176:GLU:HB2	1:B:567:LYS:HG2	1.93	0.50
1:B:851:GLN:H	1:B:851:GLN:CD	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:ASN:ND2	4:B:976:HOH:O	2.44	0.50
1:A:445:THR:OG1	1:A:457:HIS:HE1	1.94	0.49
1:B:727:HIS:NE2	1:B:829:TYR:HE2	2.09	0.49
1:B:778:ARG:NH2	4:B:1052:HOH:O	2.39	0.49
1:A:734:ARG:HD3	1:A:736:TRP:HE1	1.78	0.49
1:B:234:ALA:HB1	1:B:272:LEU:HD12	1.93	0.49
1:B:712:THR:HA	1:B:716:HIS:CD2	2.48	0.48
1:A:178:ASN:OD1	1:A:180:ASP:HB2	2.12	0.48
1:A:470:VAL:HA	1:A:636:GLY:O	2.14	0.48
1:B:82:THR:HB	1:B:84:GLU:OE2	2.14	0.48
1:A:508:PHE:HB2	1:A:524:MET:CE	2.44	0.48
1:B:602:ARG:NH1	1:B:689:ASP:OD2	2.47	0.48
1:A:551:HIS:O	1:A:554:PRO:HD2	2.12	0.48
1:A:534:VAL:CG2	1:A:579:LEU:HD11	2.44	0.48
1:A:712:THR:HA	1:A:716:HIS:HD2	1.79	0.47
1:A:709:SER:HB2	1:A:789:SER:HA	1.95	0.47
1:B:244:SER:HB2	2:B:867:TRA:OG1	2.15	0.47
1:A:398:ILE:HD13	1:A:404:CYS:SG	2.55	0.47
1:B:234:ALA:CB	1:B:272:LEU:HD12	2.44	0.47
1:B:712:THR:HA	1:B:716:HIS:HD2	1.80	0.47
1:B:851:GLN:N	1:B:851:GLN:OE1	2.32	0.47
1:A:358:ARG:NH1	1:A:358:ARG:CG	2.78	0.47
1:B:795:ASN:HA	1:B:798:GLY:O	2.15	0.47
1:B:564:THR:HG22	1:B:571:LYS:H	1.80	0.46
1:B:296:VAL:HG22	1:B:297:ASP:N	2.29	0.46
1:A:775:ASN:ND2	1:A:775:ASN:H	2.02	0.46
1:A:439:MET:CE	4:A:1105:HOH:O	2.35	0.46
1:A:460:LEU:N	1:A:461:PRO:CD	2.79	0.46
1:A:713:ASN:N	1:A:716:HIS:HD2	2.09	0.46
1:B:12:ARG:HD3	1:B:18:ALA:O	2.15	0.46
1:B:727:HIS:NE2	1:B:829:TYR:CE2	2.83	0.46
1:B:185:ALA:N	1:B:186:PRO:CD	2.78	0.46
1:B:564:THR:HG22	1:B:570:LYS:HG2	1.96	0.46
1:B:332:THR:HG23	1:B:335:LEU:H	1.81	0.46
1:A:822:THR:CG2	1:A:825:GLU:H	2.29	0.45
1:B:775:ASN:ND2	1:B:775:ASN:H	2.06	0.45
1:A:564:THR:HG22	1:A:571:LYS:N	2.14	0.45
1:B:178:ASN:HD22	1:B:178:ASN:C	2.20	0.45
1:B:682:LEU:CD2	1:B:682:LEU:N	2.79	0.45
1:B:103:ILE:O	1:B:106:LEU:HB2	2.16	0.45
1:B:616:ILE:HD12	1:B:657:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:ARG:NH2	1:B:860:ILE:O	2.50	0.45
1:A:288:ASP:OD1	1:A:344:ARG:CD	2.60	0.44
1:A:773:MET:CE	2:A:866:TRA:HG2	2.48	0.44
1:B:602:ARG:HA	1:B:602:ARG:HD3	1.83	0.44
1:B:272:LEU:HD12	1:B:272:LEU:O	2.17	0.44
1:B:93:MET:O	1:B:95:GLY:N	2.49	0.44
1:B:498:SER:OG	1:B:791:ARG:NH2	2.45	0.44
1:A:364:PRO:HB2	1:A:365:HIS:H	1.55	0.44
1:B:551:HIS:C	1:B:554:PRO:HD2	2.38	0.44
1:A:602:ARG:NH2	4:A:1018:HOH:O	2.21	0.44
1:A:254:LEU:HD21	1:A:286:MET:HE1	2.00	0.43
1:B:234:ALA:HB2	1:B:272:LEU:CD1	2.46	0.43
1:A:112:ALA:HB1	1:A:142:TYR:CD2	2.53	0.43
1:A:102:LEU:HA	1:A:102:LEU:HD12	1.86	0.43
1:A:467:ARG:NH1	4:A:1007:HOH:O	2.51	0.43
1:B:602:ARG:O	1:B:603:SER:HB2	2.17	0.43
1:B:847:ASN:ND2	1:B:847:ASN:N	2.60	0.43
1:B:796:ARG:NH1	2:B:867:TRA:OG2	2.46	0.43
1:A:785:VAL:HG23	1:A:786:VAL:N	2.33	0.43
1:A:734:ARG:HD3	1:A:736:TRP:NE1	2.33	0.43
1:A:439:MET:CB	4:A:1105:HOH:O	2.40	0.43
1:A:775:ASN:N	1:A:775:ASN:ND2	2.65	0.43
1:A:199:LEU:HD22	1:A:220:ILE:HD11	2.01	0.43
1:A:363:LEU:HB3	1:A:364:PRO:CD	2.49	0.43
1:A:822:THR:OG1	1:A:823:PRO:HD2	2.19	0.43
1:B:156:PHE:CE2	1:B:340:ARG:HG2	2.54	0.43
1:A:602:ARG:HA	1:A:602:ARG:HD3	1.87	0.42
1:B:608:THR:HG23	4:B:898:HOH:O	2.18	0.42
1:B:178:ASN:HB3	1:B:181:ASP:OD2	2.19	0.42
1:B:822:THR:N	1:B:825:GLU:HG3	2.29	0.42
1:B:2:LEU:HD12	1:B:2:LEU:HA	1.79	0.42
1:B:534:VAL:CG2	1:B:579:LEU:HD11	2.49	0.42
1:B:309:VAL:O	1:B:311:PRO:HD3	2.19	0.42
1:A:839:ASP:O	1:A:842:ARG:HD3	2.19	0.42
1:A:704:GLU:OE2	1:A:779:VAL:HG22	2.19	0.42
1:B:498:SER:O	1:B:501:ARG:HD3	2.20	0.42
1:A:564:THR:HG21	4:A:919:HOH:O	2.20	0.42
1:B:602:ARG:NH2	4:B:990:HOH:O	2.46	0.42
1:A:12:ARG:HD2	1:A:19:PRO:HA	2.01	0.42
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.91	0.42
1:A:820:LEU:HD23	1:A:820:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HB2	1:A:567:LYS:HD2	2.02	0.42
1:A:100:HIS:N	1:A:101:PRO:CD	2.83	0.41
1:A:37:PRO:HA	1:A:38:PRO:HD3	1.91	0.41
1:B:723:LEU:HG	1:B:833:VAL:HG21	2.02	0.41
1:B:534:VAL:HG21	1:B:579:LEU:HD11	2.02	0.41
1:B:731:LEU:HA	1:B:732:PRO:HD3	1.82	0.41
1:B:321:THR:CG2	1:B:323:GLU:HG3	2.50	0.41
1:B:56:GLY:HA2	1:B:95:GLY:O	2.20	0.41
1:B:41:GLU:O	1:B:45:LEU:HG	2.20	0.41
1:A:809:GLU:H	1:A:809:GLU:CD	2.21	0.41
1:A:453:ASP:O	1:A:456:THR:HB	2.20	0.41
1:B:237:GLY:O	1:B:275:GLY:HA2	2.20	0.41
1:B:182:LEU:CD2	1:B:201:MET:HE2	2.49	0.41
1:A:363:LEU:HB3	1:A:364:PRO:HD2	2.02	0.41
1:A:550:VAL:HG22	1:A:595:LEU:HD23	2.02	0.41
1:B:460:LEU:N	1:B:461:PRO:CD	2.84	0.41
1:A:415:ASP:OD1	1:A:415:ASP:N	2.52	0.41
1:A:502:PHE:HB3	1:A:504:ILE:O	2.21	0.41
1:B:524:MET:HA	1:B:525:PRO:HD3	1.98	0.41
1:A:23:ASP:C	1:A:23:ASP:OD1	2.59	0.40
1:A:287:GLU:OE2	1:A:338:GLU:OE1	2.40	0.40
1:A:321:THR:HG21	1:A:323:GLU:CD	2.41	0.40
1:A:534:VAL:HG23	1:A:579:LEU:HD11	2.03	0.40
1:A:82:THR:HG22	4:A:1033:HOH:O	2.21	0.40
1:B:93:MET:C	1:B:95:GLY:H	2.23	0.40
1:B:727:HIS:CE1	1:B:829:TYR:HE2	2.39	0.40
1:B:108:ASP:OD1	1:B:108:ASP:C	2.60	0.40
1:B:42:GLU:HG2	1:B:42:GLU:H	1.26	0.40
1:A:614:GLU:N	1:A:615:PRO:HD2	2.37	0.40
1:A:528:MET:HA	1:A:529:PRO:HD3	1.77	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	860/865 (99%)	831 (97%)	26 (3%)	3 (0%)	46	63
1	B	860/865 (99%)	828 (96%)	31 (4%)	1 (0%)	56	74
All	All	1720/1730 (99%)	1659 (96%)	57 (3%)	4 (0%)	52	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	PRO
1	A	94	GLN
1	A	708	GLY
1	B	708	GLY

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	690/692 (100%)	654 (95%)	36 (5%)	29	45
1	B	690/692 (100%)	646 (94%)	44 (6%)	22	34
All	All	1380/1384 (100%)	1300 (94%)	80 (6%)	25	39

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	46	LEU
1	A	59	GLU
1	A	81	LEU
1	A	82	THR
1	A	94	GLN
1	A	102	LEU
1	A	133	GLU
1	A	172	LYS

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Mol	Chain	Res	Type
1	A	180	ASP
1	A	196	LEU
1	A	221	LYS
1	A	268	ARG
1	A	277	LYS
1	A	307	ILE
1	A	327	THR
1	A	344	ARG
1	A	358	ARG
1	A	391	ARG
1	A	414	GLN
1	A	431	LEU
1	A	467	ARG
1	A	546	LEU
1	A	588	LYS
1	A	590	GLU
1	A	601	GLU
1	A	602	ARG
1	A	644	ARG
1	A	773	MET
1	A	775	ASN
1	A	779	VAL
1	A	785	VAL
1	A	786	VAL
1	A	797	LEU
1	A	834	ASP
1	A	847	ASN
1	B	2	LEU
1	B	12	ARG
1	B	42	GLU
1	B	46	LEU
1	B	52	ARG
1	B	89	LEU
1	B	106	LEU
1	B	133	GLU
1	B	157	LEU
1	B	178	ASN
1	B	196	LEU
1	B	221	LYS
1	B	253	VAL
1	B	272	LEU
1	B	277	LYS

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Mol	Chain	Res	Type
1	B	292	LEU
1	B	340	ARG
1	B	391	ARG
1	B	399	ARG
1	B	414	GLN
1	B	431	LEU
1	B	533	LEU
1	B	549	LEU
1	B	555	LEU
1	B	563	LEU
1	B	564	THR
1	B	602	ARG
1	B	603	SER
1	B	644	ARG
1	B	677	ILE
1	B	682	LEU
1	B	694	LEU
1	B	724	LEU
1	B	748	LEU
1	B	763	ARG
1	B	775	ASN
1	B	779	VAL
1	B	797	LEU
1	B	805	LEU
1	B	817	ILE
1	B	825	GLU
1	B	847	ASN
1	B	849	LEU
1	B	850	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	213	GLN
1	A	228	GLN
1	A	386	GLN
1	A	457	HIS
1	A	466	ASN
1	A	623	ASN
1	A	646	GLN
1	A	716	HIS

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Mol	Chain	Res	Type
1	A	775	ASN
1	A	832	GLN
1	A	845	ASN
1	A	847	ASN
1	A	848	GLN
1	B	148	GLN
1	B	178	ASN
1	B	365	HIS
1	B	371	GLN
1	B	466	ASN
1	B	623	ASN
1	B	646	GLN
1	B	654	ASN
1	B	698	GLN
1	B	716	HIS
1	B	775	ASN
1	B	832	GLN
1	B	845	ASN
1	B	847	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	TRA	A	866	-	3,11,11	1.63	1 (33%)	3,14,14	3.49	3 (100%)
3	F3S	A	868	1	0,9,9	0.00	-	0,15,15	0.00	-
2	TRA	B	867	-	3,11,11	1.87	1 (33%)	3,14,14	2.87	3 (100%)
3	F3S	B	869	1	0,9,9	0.00	-	0,15,15	0.00	-

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	TRA	A	866	-	-	0/4/12/12	0/0/0/0
3	F3S	A	868	1	-	0/0/24/24	0/0/3/3
2	TRA	B	867	-	-	0/4/12/12	0/0/0/0
3	F3S	B	869	1	-	0/0/24/24	0/0/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	867	TRA	CA-CB	-2.56	1.32	1.34
2	A	866	TRA	CA-CB	-2.31	1.32	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	866	TRA	CAC-CA-CB	-4.66	116.68	127.14
2	B	867	TRA	CAC-CA-CB	-3.52	119.23	127.14
2	A	866	TRA	CGC-CG-CB	-2.77	107.06	114.00
2	A	866	TRA	CG-CB-CA	-2.67	118.95	125.70
2	B	867	TRA	CG-CB-CA	-2.57	119.21	125.70
2	B	867	TRA	CGC-CG-CB	-2.39	108.00	114.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	866	TRA	2	0
2	B	867	TRA	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	862/865 (99%)	-0.69	15 (1%)	73	72	17, 32, 71, 97	0
1	B	862/865 (99%)	-0.74	12 (1%)	78	77	18, 32, 66, 96	0
All	All	1724/1730 (99%)	-0.72	27 (1%)	74	74	17, 32, 68, 97	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	GLU	7.7
1	A	377	GLU	7.1
1	B	376	ALA	6.4
1	B	375	VAL	4.7
1	A	138	ALA	4.4
1	B	374	ASP	4.4
1	B	378	SER	4.2
1	B	379	ASP	4.0
1	A	376	ALA	3.9
1	A	374	ASP	3.9
1	B	728	LYS	3.7
1	A	373	LYS	3.7
1	A	365	HIS	3.1
1	A	375	VAL	3.0
1	B	373	LYS	2.9
1	B	371	GLN	2.8
1	A	379	ASP	2.8
1	A	728	LYS	2.8
1	B	1	MET	2.7
1	A	378	SER	2.6
1	A	75	GLU	2.5
1	A	367	ASP	2.5
1	A	137	LYS	2.4
1	A	862	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	365	HIS	2.3
1	B	636	GLY	2.1
1	A	146	VAL	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	TRA	A	866	12/12	0.97	0.12	0.89	18,26,31,37	0
2	TRA	B	867	12/12	0.97	0.11	0.77	25,31,40,65	0
3	F3S	A	868	7/7	0.98	0.06	-1.07	19,26,30,30	0
3	F3S	B	869	7/7	0.98	0.04	-2.32	21,26,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.