W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:21 AM GMT

PDB ID	:	3EAD
Title	:	Crystal structure of CALX-CBD1
Authors	:	Zheng, L.; Wang, M.
Deposited on	:	2008-08-25
Resolution	:	2.25 Å(reported)

The following versions of software and data (see references (i)) 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 2.25 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.
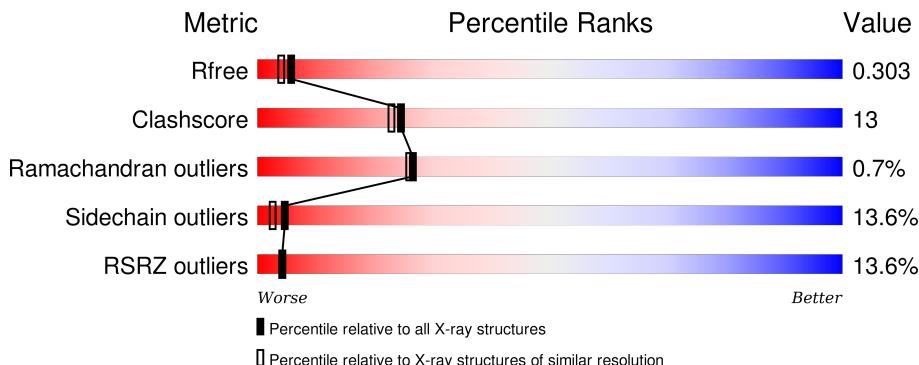
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	137	12% 58% 15% 9% 19%
1	B	137	8% 60% 18% 5% • 17%
1	C	137	8% 53% 25% • 18%
1	D	137	17% 58% 18% • • 19%
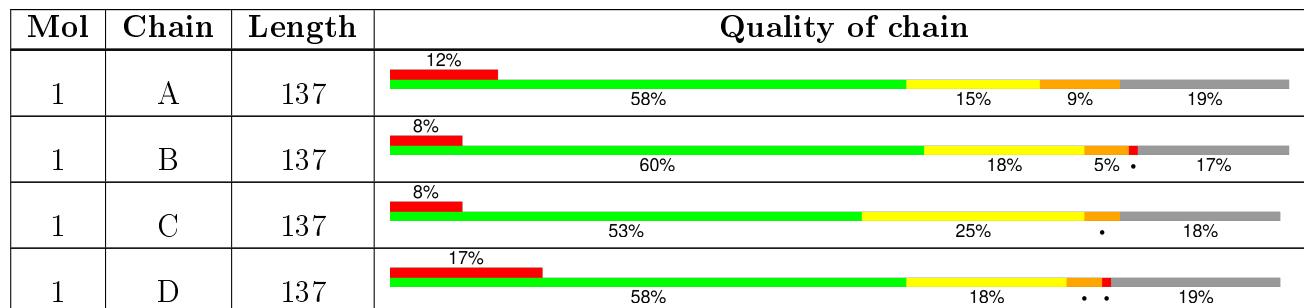
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	A	1002	-	-	-	X
2	CA	D	1002	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3693 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 Na/Ca exchange protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			886	560	143	177	6			
1	B	114	Total	C	N	O	S	0	0	0
			908	574	148	180	6			
1	C	112	Total	C	N	O	S	0	0	0
			896	566	146	178	6			
1	D	111	Total	C	N	O	S	0	0	0
			886	560	143	177	6			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Ca	0	0
			4	4		
2	A	4	Total	Ca	0	0
			4	4		
2	D	4	Total	Ca	0	0
			4	4		
2	C	4	Total	Ca	0	0
			4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
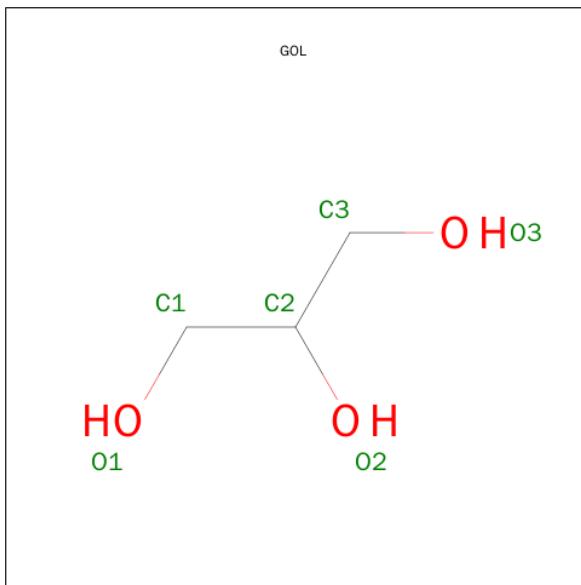
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total C O 6 3 3			0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total O 31 31		0	0
4	B	27	Total O 27 27		0	0
4	C	25	Total O 25 25		0	0
4	D	12	Total O 12 12		0	0

3 Residue-property plots ⓘ

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: Na/Ca exchange protein
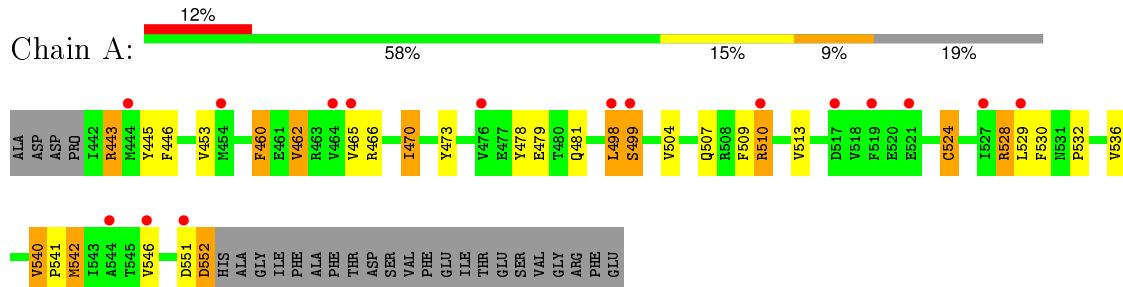
- Molecule 1: Na/Ca exchange protein

- Molecule 1: Na/Ca exchange protein

- Molecule 1: Na/Ca exchange protein

V536 K537 V540 P541 T545 V546 M547 I548 L549 D550 D551 D552 HIS ALA GLY ILE PHE ALA PHE THR ASP SER VAL PHE GLU ILE THR GLU SER VAL GLY ARG PHE GLU
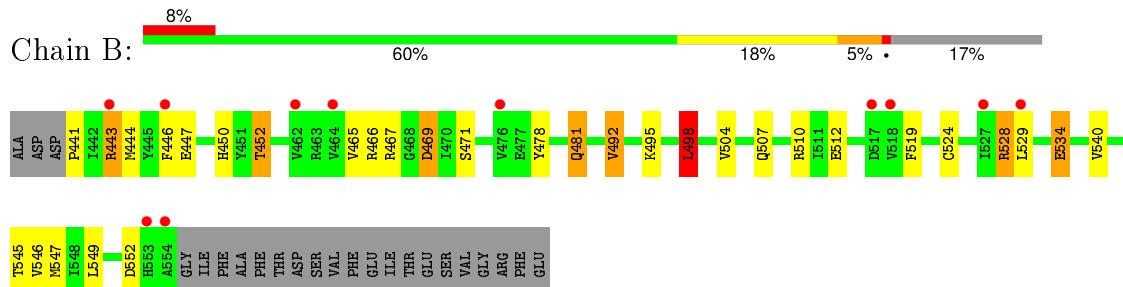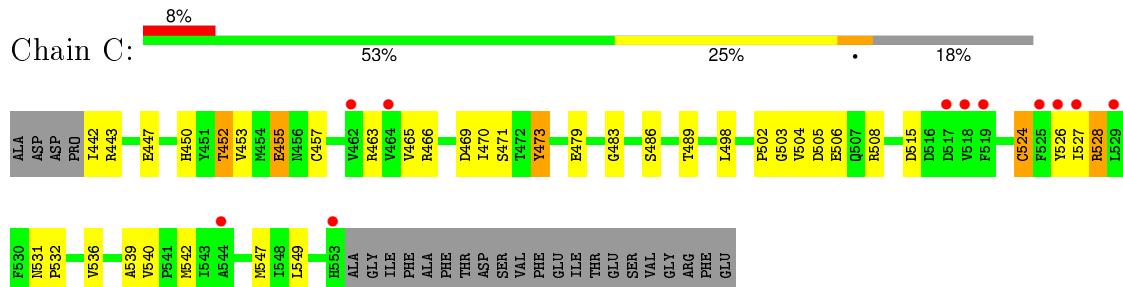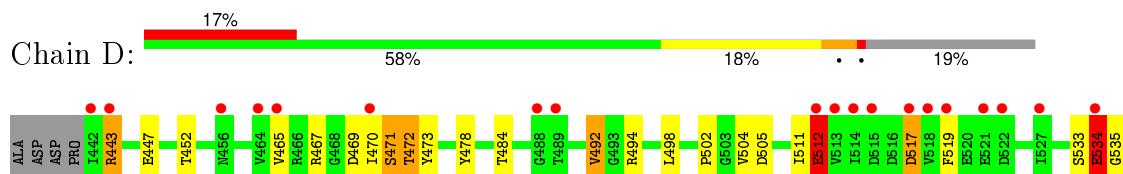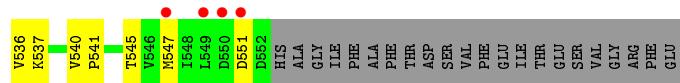
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.37Å 73.72Å 129.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.59 – 2.25 19.58 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.5 (19.59-2.25) 94.5 (19.58-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.269 0.260 , 0.303	Depositor DCC
R_{free} test set	1340 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 29.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 26173 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3693	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GOL, CA

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	1.19	8/904 (0.9%)	0.98	3/1223 (0.2%)
1	B	0.89	1/928 (0.1%)	0.93	3/1256 (0.2%)
1	C	0.92	1/915 (0.1%)	0.87	1/1238 (0.1%)
1	D	0.93	4/904 (0.4%)	0.81	2/1223 (0.2%)
All	All	0.99	14/3651 (0.4%)	0.90	9/4940 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	524	CYS	CB-SG	-8.64	1.67	1.82
1	A	552	ASP	CG-OD1	8.12	1.44	1.25
1	D	512	GLU	CD-OE2	7.06	1.33	1.25
1	A	542	MET	CG-SD	6.98	1.99	1.81
1	A	462	VAL	CB-CG1	6.94	1.67	1.52
1	D	517	ASP	CG-OD1	6.78	1.41	1.25
1	A	552	ASP	CB-CG	6.28	1.65	1.51
1	D	512	GLU	CG-CD	6.12	1.61	1.51
1	A	460	PHE	CE1-CZ	5.98	1.48	1.37
1	D	551	ASP	CG-OD1	5.72	1.38	1.25
1	A	478	TYR	CD2-CE2	5.57	1.47	1.39
1	A	509	PHE	CD2-CE2	-5.33	1.28	1.39
1	A	524	CYS	CB-SG	-5.24	1.73	1.81
1	B	447	GLU	CD-OE2	-5.15	1.20	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	551	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	447	GLU	OE1-CD-OE2	-6.46	115.55	123.30
1	A	528	ARG	NE-CZ-NH2	-6.42	117.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	447	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	A	498	LEU	CA-CB-CG	5.68	128.35	115.30
1	B	498	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	542	MET	CG-SD-CE	-5.34	91.66	100.20
1	C	528	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	528	ARG	CB-CA-C	-5.23	99.94	110.40

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	886	0	837	34	0
1	B	908	0	857	21	0
1	C	896	0	844	38	0
1	D	886	0	837	16	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	6	0	8	0	0
4	A	31	0	0	1	0
4	B	27	0	0	1	0
4	C	25	0	0	1	0
4	D	12	0	0	0	0
All	All	3693	0	3383	90	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 13.

All (90) 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:C:549:LEU:HB3	1:D:443:ARG:NH1	1.69	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ARG:HG2	1:A:443:ARG:HH11	1.22	1.03
1:A:542:MET:HE3	1:C:483:GLY:HA2	1.54	0.88
1:A:510:ARG:H	1:A:510:ARG:HD2	1.39	0.87
1:A:470:ILE:O	1:A:470:ILE:HG23	1.72	0.87
1:C:469:ASP:OD1	1:C:471:SER:HB3	1.75	0.85
1:C:470:ILE:O	1:C:470:ILE:HG22	1.79	0.82
1:A:542:MET:HE3	1:C:483:GLY:CA	2.12	0.79
1:A:443:ARG:CG	1:A:443:ARG:HH11	1.95	0.79
1:A:443:ARG:HG2	1:A:443:ARG:NH1	1.96	0.77
1:A:540:VAL:O	1:B:452:THR:HG21	1.85	0.77
1:A:470:ILE:O	1:A:470:ILE:CG2	2.32	0.76
1:C:452:THR:HG21	1:D:540:VAL:O	1.89	0.71
1:B:450:HIS:ND1	1:B:545:THR:HG23	2.06	0.70
1:D:533:SER:O	1:D:534:GLU:C	2.30	0.70
1:A:542:MET:HE2	1:C:526:TYR:CE1	2.27	0.69
1:A:542:MET:CE	1:C:526:TYR:HE1	2.06	0.68
1:A:542:MET:HE2	1:C:526:TYR:HE1	1.59	0.68
1:C:471:SER:O	1:C:502:PRO:HB3	1.95	0.67
1:A:443:ARG:HD3	1:B:549:LEU:HD13	1.77	0.67
1:C:549:LEU:HB3	1:D:443:ARG:HH12	1.55	0.66
1:A:510:ARG:HD2	1:A:510:ARG:N	2.10	0.66
1:C:470:ILE:O	1:C:470:ILE:CG2	2.45	0.65
1:A:542:MET:CE	1:C:483:GLY:CA	2.75	0.64
1:C:470:ILE:HG22	1:C:503:GLY:H	1.64	0.63
1:A:453:VAL:HG11	1:A:513:VAL:HG21	1.80	0.62
1:A:532:PRO:HB2	1:A:536:VAL:HB	1.84	0.59
1:C:450:HIS:NE2	1:C:452:THR:HG22	2.18	0.59
1:C:442:ILE:HG21	1:C:536:VAL:HG22	1.84	0.59
1:D:472:THR:OG1	1:D:473:TYR:N	2.35	0.58
1:C:528:ARG:NH2	4:C:146:HOH:O	2.37	0.58
1:A:479:GLU:OE2	1:A:528:ARG:NH1	2.37	0.57
1:A:507:GLN:NE2	4:A:1032:HOH:O	2.37	0.57
1:B:492:VAL:HG13	1:B:512:GLU:HB3	1.85	0.57
1:C:442:ILE:CG2	1:C:536:VAL:HG22	2.35	0.56
1:C:453:VAL:HG22	1:C:457:CYS:SG	2.46	0.55
1:A:541:PRO:HD3	1:B:452:THR:HG21	1.89	0.55
1:C:455:GLU:HG3	1:C:515:ASP:HA	1.88	0.54
1:B:441:PRO:O	1:B:443:ARG:HG2	2.08	0.54
1:A:446:PHE:CE2	1:A:462:VAL:CG1	2.91	0.54
1:A:541:PRO:HD3	1:B:452:THR:CG2	2.38	0.54
1:C:443:ARG:HE	1:C:539:ALA:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:PHE:HE2	1:A:462:VAL:CG1	2.20	0.53
1:B:444:MET:HA	1:B:465:VAL:O	2.09	0.52
1:C:470:ILE:HD13	1:C:505:ASP:HB3	1.92	0.51
1:D:478:TYR:OH	1:D:494:ARG:NH2	2.43	0.51
1:B:481:GLN:OE1	1:B:528:ARG:HG3	2.10	0.51
1:A:542:MET:CE	1:C:483:GLY:HA3	2.41	0.50
1:C:506:GLU:OE2	1:C:508:ARG:NH2	2.45	0.50
1:C:473:TYR:C	1:C:473:TYR:CD2	2.84	0.50
1:B:469:ASP:OD2	1:B:471:SER:HB3	2.11	0.50
1:A:551:ASP:N	1:A:551:ASP:OD1	2.44	0.50
1:C:470:ILE:CD1	1:C:505:ASP:HB3	2.42	0.49
1:A:524:CYS:HA	1:A:546:VAL:O	2.12	0.49
1:D:533:SER:O	1:D:534:GLU:O	2.30	0.49
1:B:481:GLN:OE1	1:B:528:ARG:HD2	2.13	0.49
1:A:542:MET:HE1	1:C:483:GLY:HA3	1.95	0.47
1:A:460:PHE:O	1:A:510:ARG:HA	2.14	0.47
1:D:534:GLU:O	1:D:536:VAL:N	2.45	0.46
1:A:446:PHE:HE2	1:A:462:VAL:HG11	1.80	0.46
1:D:492:VAL:HG13	1:D:512:GLU:HB2	1.96	0.46
1:C:452:THR:HG21	1:D:541:PRO:HD3	1.98	0.46
1:B:507:GLN:NE2	4:B:46:HOH:O	2.47	0.46
1:A:446:PHE:CE2	1:A:462:VAL:HG11	2.52	0.45
1:B:519:PHE:HA	1:B:552:ASP:HB2	1.99	0.44
1:D:469:ASP:OD2	1:D:471:SER:OG	2.30	0.44
1:B:450:HIS:NE2	1:B:452:THR:HG22	2.32	0.44
1:B:446:PHE:CE1	1:B:529:LEU:HG	2.53	0.44
1:C:453:VAL:CG2	1:C:457:CYS:SG	3.06	0.44
1:B:524:CYS:HA	1:B:546:VAL:O	2.17	0.44
1:C:450:HIS:CD2	1:C:452:THR:HG22	2.52	0.44
1:C:452:THR:CG2	1:D:541:PRO:HD3	2.47	0.44
1:A:453:VAL:CG1	1:A:513:VAL:HG21	2.47	0.44
1:D:467:ARG:NH1	1:D:505:ASP:HB2	2.33	0.44
1:A:473:TYR:CE1	1:A:499:SER:HB3	2.53	0.44
1:C:452:THR:HB	1:C:547:MET:HB3	1.99	0.43
1:B:478:TYR:HA	1:B:528:ARG:O	2.17	0.43
1:C:549:LEU:HB3	1:D:443:ARG:HH11	1.68	0.43
1:A:542:MET:CE	1:C:526:TYR:CE1	2.92	0.43
1:C:447:GLU:O	1:C:463:ARG:HD3	2.19	0.43
1:D:494:ARG:HD3	1:D:511:ILE:HD13	2.00	0.42
1:D:443:ARG:HB3	1:D:537:LYS:O	2.18	0.42
1:B:478:TYR:CE1	1:B:498:LEU:HD13	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:HIS:CD2	1:B:452:THR:HG22	2.56	0.41
1:B:452:THR:HB	1:B:547:MET:HB3	2.03	0.41
1:B:534:GLU:H	1:B:534:GLU:HG2	1.48	0.41
1:C:531:ASN:N	1:C:532:PRO:CD	2.84	0.41
1:C:479:GLU:OE2	1:C:528:ARG:NH1	2.51	0.41
1:C:527:ILE:HG21	1:C:527:ILE:HD13	1.79	0.40
1:A:529:LEU:O	1:A:530:PHE:HB3	2.20	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	109/137 (80%)	103 (94%)	6 (6%)	0	100	100
1	B	112/137 (82%)	107 (96%)	5 (4%)	0	100	100
1	C	110/137 (80%)	105 (96%)	5 (4%)	0	100	100
1	D	109/137 (80%)	102 (94%)	4 (4%)	3 (3%)	6	3
All	All	440/548 (80%)	417 (95%)	20 (4%)	3 (1%)	26	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	534	GLU
1	D	502	PRO
1	D	535	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	97/118 (82%)	85 (88%)	12 (12%)	6	4
1	B	99/118 (84%)	86 (87%)	13 (13%)	5	3
1	C	98/118 (83%)	86 (88%)	12 (12%)	6	4
1	D	97/118 (82%)	81 (84%)	16 (16%)	3	1
All	All	391/472 (83%)	338 (86%)	53 (14%)	5	2

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	ARG
1	A	445	TYR
1	A	465	VAL
1	A	466	ARG
1	A	470	ILE
1	A	481	GLN
1	A	498	LEU
1	A	499	SER
1	A	504	VAL
1	A	510	ARG
1	A	540	VAL
1	A	552	ASP
1	B	443	ARG
1	B	452	THR
1	B	466	ARG
1	B	467	ARG
1	B	469	ASP
1	B	481	GLN
1	B	492	VAL
1	B	495	LYS
1	B	498	LEU
1	B	504	VAL
1	B	510	ARG
1	B	534	GLU
1	B	540	VAL
1	C	452	THR
1	C	455	GLU
1	C	465	VAL

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Mol	Chain	Res	Type
1	C	466	ARG
1	C	473	TYR
1	C	486	SER
1	C	489	THR
1	C	498	LEU
1	C	504	VAL
1	C	524	CYS
1	C	540	VAL
1	C	542	MET
1	D	443	ARG
1	D	452	THR
1	D	465	VAL
1	D	470	ILE
1	D	471	SER
1	D	472	THR
1	D	484	THR
1	D	492	VAL
1	D	498	LEU
1	D	504	VAL
1	D	512	GLU
1	D	517	ASP
1	D	519	PHE
1	D	534	GLU
1	D	545	THR
1	D	547	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	HIS
1	A	481	GLN
1	A	507	GLN
1	B	507	GLN
1	C	481	GLN
1	C	553	HIS
1	D	481	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)

Of 17 ligands modelled in this entry, 16 are monoatomic - leaving 1 for Mogul analysis.

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	#$|Z| > 2$
3	GOL	A	1	-	5,5,5	0.35	0	5,5,5	0.69	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
3	GOL	A	1	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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(Å²)	Q<0.9
1	A	111/137 (81%)	0.69	16 (14%)	3	4	38, 46, 54, 60	0
1	B	114/137 (83%)	0.47	11 (9%)	10	11	43, 48, 54, 59	0
1	C	112/137 (81%)	0.43	11 (9%)	10	10	40, 48, 55, 58	0
1	D	111/137 (81%)	1.07	23 (20%)	1	1	44, 50, 57, 61	0
All	All	448/548 (81%)	0.67	61 (13%)	4	4	38, 48, 56, 61	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	517	ASP	7.6
1	A	517	ASP	7.2
1	D	518	VAL	6.7
1	C	527	ILE	6.6
1	C	553	HIS	5.7
1	D	519	PHE	5.3
1	D	551	ASP	4.5
1	A	519	PHE	4.4
1	D	550	ASP	3.9
1	B	553	HIS	3.9
1	B	554	ALA	3.8
1	B	464	VAL	3.8
1	D	515	ASP	3.5
1	A	529	LEU	3.5
1	D	527	ILE	3.5
1	B	527	ILE	3.4
1	D	488	GLY	3.2
1	B	443	ARG	3.2
1	A	527	ILE	3.1
1	B	529	LEU	3.1
1	D	464	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	462	VAL	3.1
1	A	498	LEU	2.9
1	C	462	VAL	2.9
1	C	464	VAL	2.8
1	D	456	ASN	2.8
1	A	544	ALA	2.8
1	D	549	LEU	2.7
1	C	544	ALA	2.7
1	C	517	ASP	2.6
1	A	465	VAL	2.6
1	C	525	PHE	2.5
1	A	464	VAL	2.5
1	D	534	GLU	2.5
1	A	476	VAL	2.5
1	C	518	VAL	2.5
1	A	551	ASP	2.5
1	C	526	TYR	2.5
1	A	510	ARG	2.4
1	A	444	MET	2.4
1	D	465	VAL	2.4
1	D	547	MET	2.3
1	B	446	PHE	2.3
1	D	442	ILE	2.3
1	A	454	MET	2.3
1	B	518	VAL	2.3
1	D	489	THR	2.3
1	B	476	VAL	2.3
1	D	512	GLU	2.3
1	D	521	GLU	2.2
1	B	517	ASP	2.2
1	D	522	ASP	2.2
1	A	521	GLU	2.1
1	A	499	SER	2.1
1	C	519	PHE	2.1
1	D	514	ILE	2.1
1	D	513	VAL	2.1
1	C	529	LEU	2.1
1	D	470	ILE	2.1
1	A	546	VAL	2.1
1	D	443	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	A	1002	1/1	0.94	0.26	2.48	70,70,70,70	0
2	CA	D	1002	1/1	0.94	0.32	2.10	83,83,83,83	0
2	CA	B	1002	1/1	0.96	0.14	0.36	46,46,46,46	0
3	GOL	A	1	6/6	0.60	0.18	-0.01	59,61,64,65	0
2	CA	B	1001	1/1	0.94	0.10	-0.07	53,53,53,53	0
2	CA	C	1002	1/1	0.98	0.13	-0.13	47,47,47,47	0
2	CA	A	1004	1/1	0.96	0.10	-0.97	75,75,75,75	0
2	CA	D	1004	1/1	0.82	0.22	-1.11	90,90,90,90	0
2	CA	A	1003	1/1	0.89	0.11	-1.20	68,68,68,68	0
2	CA	D	1003	1/1	0.74	0.18	-1.39	92,92,92,92	0
2	CA	B	1004	1/1	0.90	0.06	-1.86	58,58,58,58	0
2	CA	C	1004	1/1	0.96	0.05	-1.88	62,62,62,62	0
2	CA	C	1003	1/1	0.98	0.02	-1.97	50,50,50,50	0
2	CA	B	1003	1/1	0.96	0.05	-2.01	49,49,49,49	0
2	CA	C	1001	1/1	0.98	0.15	-	52,52,52,52	0
2	CA	A	1001	1/1	0.93	0.22	-	69,69,69,69	0
2	CA	D	1001	1/1	0.81	0.13	-	83,83,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.