Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 10:52 AM EDT

PDB ID	:	5FBK
Title	:	Crystal structure of the extracellular domain of human calcium sensing receptor
Authors	:	Zhang, T.; Zhang, C.; Miller, C.L.; Zou, J.; Moremen, K.W.; Brown, E.M.; Yang, J.J.; Hu, J.
Deposited on	:	2015-12-14
Resolution	:	2.10 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 (i)) were used in the production of this report:

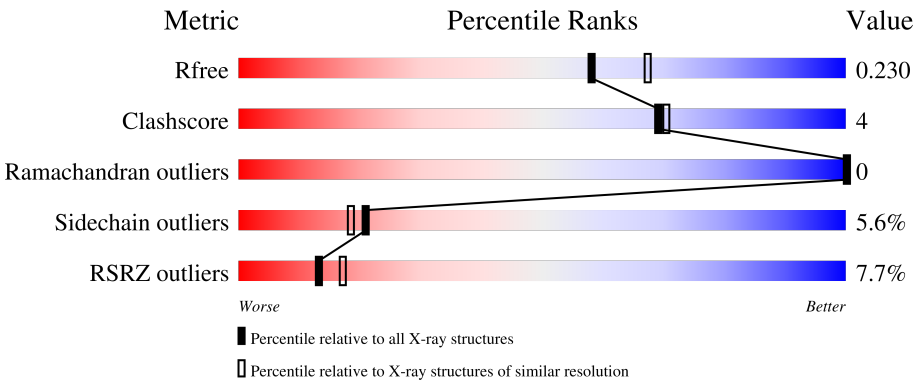
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	568	8% 79% 5% • 14%
1	B	568	5% 73% 7% • 18%

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
3	NAG	B	605	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7901 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 Extracellular calcium-sensing receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3778	2424	631	710	13	0	0	0
1	B	467	3639	2335	615	677	12	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP P41180
A	-25	ARG	-	expression tag	UNP P41180
A	-24	LEU	-	expression tag	UNP P41180
A	-23	LEU	-	expression tag	UNP P41180
A	-22	THR	-	expression tag	UNP P41180
A	-21	ALA	-	expression tag	UNP P41180
A	-20	LEU	-	expression tag	UNP P41180
A	-19	PHE	-	expression tag	UNP P41180
A	-18	ALA	-	expression tag	UNP P41180
A	-17	TYR	-	expression tag	UNP P41180
A	-16	PHE	-	expression tag	UNP P41180
A	-15	ILE	-	expression tag	UNP P41180
A	-14	VAL	-	expression tag	UNP P41180
A	-13	ALA	-	expression tag	UNP P41180
A	-12	LEU	-	expression tag	UNP P41180
A	-11	ILE	-	expression tag	UNP P41180
A	-10	LEU	-	expression tag	UNP P41180
A	-9	ALA	-	expression tag	UNP P41180
A	-8	PHE	-	expression tag	UNP P41180
A	-7	SER	-	expression tag	UNP P41180
A	-6	VAL	-	expression tag	UNP P41180
A	-5	SER	-	expression tag	UNP P41180
A	-4	ALA	-	expression tag	UNP P41180
A	-3	LYS	-	expression tag	UNP P41180
A	-2	SER	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P41180
A	0	HIS	-	expression tag	UNP P41180
A	1	HIS	-	expression tag	UNP P41180
A	2	HIS	-	expression tag	UNP P41180
A	3	HIS	-	expression tag	UNP P41180
A	4	HIS	-	expression tag	UNP P41180
A	5	HIS	-	expression tag	UNP P41180
A	6	HIS	-	expression tag	UNP P41180
A	7	HIS	-	expression tag	UNP P41180
A	8	SER	-	expression tag	UNP P41180
A	9	ALA	-	expression tag	UNP P41180
A	10	TRP	-	expression tag	UNP P41180
A	11	SER	-	expression tag	UNP P41180
A	12	HIS	-	expression tag	UNP P41180
A	13	PRO	-	expression tag	UNP P41180
A	14	GLN	-	expression tag	UNP P41180
A	15	PHE	-	expression tag	UNP P41180
A	16	GLU	-	expression tag	UNP P41180
A	17	LYS	-	expression tag	UNP P41180
A	18	GLU	-	expression tag	UNP P41180
A	19	PHE	-	expression tag	UNP P41180
B	-26	MET	-	initiating methionine	UNP P41180
B	-25	ARG	-	expression tag	UNP P41180
B	-24	LEU	-	expression tag	UNP P41180
B	-23	LEU	-	expression tag	UNP P41180
B	-22	THR	-	expression tag	UNP P41180
B	-21	ALA	-	expression tag	UNP P41180
B	-20	LEU	-	expression tag	UNP P41180
B	-19	PHE	-	expression tag	UNP P41180
B	-18	ALA	-	expression tag	UNP P41180
B	-17	TYR	-	expression tag	UNP P41180
B	-16	PHE	-	expression tag	UNP P41180
B	-15	ILE	-	expression tag	UNP P41180
B	-14	VAL	-	expression tag	UNP P41180
B	-13	ALA	-	expression tag	UNP P41180
B	-12	LEU	-	expression tag	UNP P41180
B	-11	ILE	-	expression tag	UNP P41180
B	-10	LEU	-	expression tag	UNP P41180
B	-9	ALA	-	expression tag	UNP P41180
B	-8	PHE	-	expression tag	UNP P41180
B	-7	SER	-	expression tag	UNP P41180
B	-6	VAL	-	expression tag	UNP P41180

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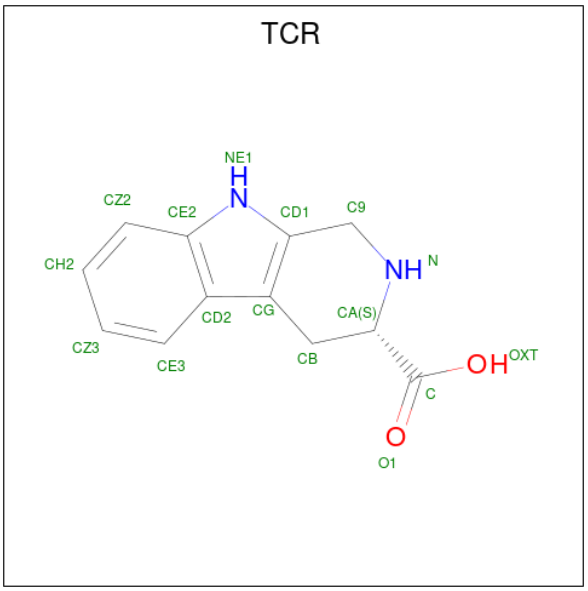
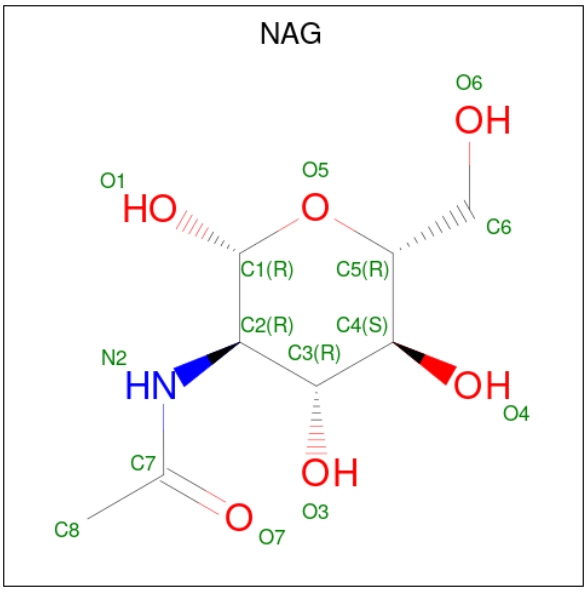
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	SER	-	expression tag	UNP P41180
B	-4	ALA	-	expression tag	UNP P41180
B	-3	LYS	-	expression tag	UNP P41180
B	-2	SER	-	expression tag	UNP P41180
B	-1	MET	-	expression tag	UNP P41180
B	0	HIS	-	expression tag	UNP P41180
B	1	HIS	-	expression tag	UNP P41180
B	2	HIS	-	expression tag	UNP P41180
B	3	HIS	-	expression tag	UNP P41180
B	4	HIS	-	expression tag	UNP P41180
B	5	HIS	-	expression tag	UNP P41180
B	6	HIS	-	expression tag	UNP P41180
B	7	HIS	-	expression tag	UNP P41180
B	8	SER	-	expression tag	UNP P41180
B	9	ALA	-	expression tag	UNP P41180
B	10	TRP	-	expression tag	UNP P41180
B	11	SER	-	expression tag	UNP P41180
B	12	HIS	-	expression tag	UNP P41180
B	13	PRO	-	expression tag	UNP P41180
B	14	GLN	-	expression tag	UNP P41180
B	15	PHE	-	expression tag	UNP P41180
B	16	GLU	-	expression tag	UNP P41180
B	17	LYS	-	expression tag	UNP P41180
B	18	GLU	-	expression tag	UNP P41180
B	19	PHE	-	expression tag	UNP P41180

- Molecule 2 is CYCLOMETHYLTRYPTOPHAN (three-letter code: TCR) (formula: $C_{12}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	16	12	2	2	0	0
			Total	C	N	O		
2	B	1	16	12	2	2	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0

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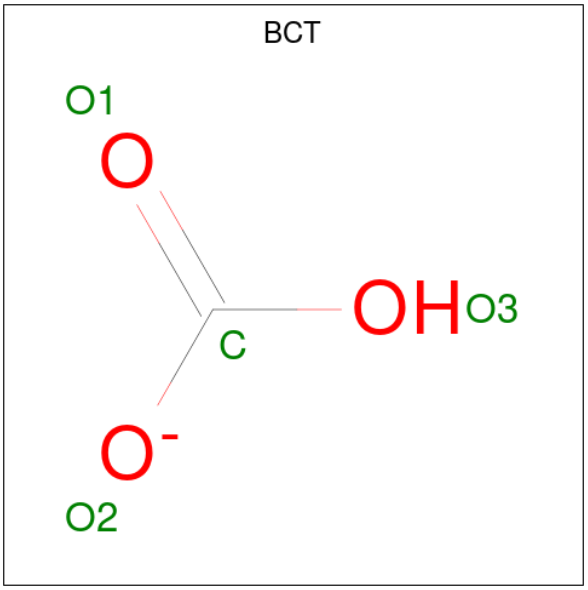
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Cl 3 3	0	0
4	B	3	Total Cl 3 3	0	0

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	1	3	0	0
			Total	C	O		
5	B	1	4	1	3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0
			Total	Mg		
6	B	2	2	2	0	0

- Molecule 7 is water.

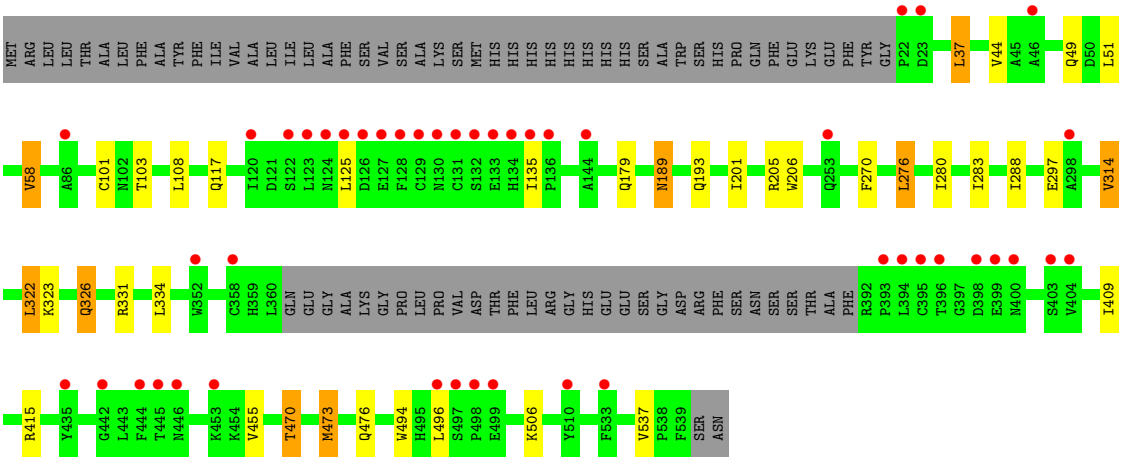
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	153	153	153	0	0
			Total	O		
7	B	170	170	170	0	0

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.

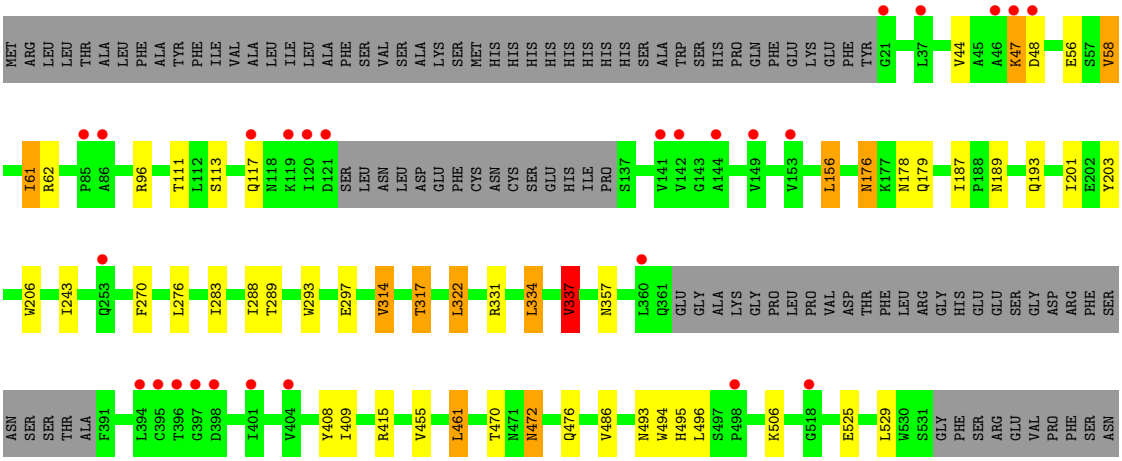
• Molecule 1: Extracellular calcium-sensing receptor

Chain A:



• Molecule 1: Extracellular calcium-sensing receptor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.87Å 82.92Å 94.26Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	37.77 – 2.10 37.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.77-2.10) 99.8 (37.77-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.190 , 0.223 0.197 , 0.230	Depositor DCC
R_{free} test set	2000 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7901	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, CL, TCR, MG, NAG, CSO

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	0/3854	0.66	1/5241 (0.0%)
1	B	0.52	0/3712	0.69	2/5042 (0.0%)
All	All	0.50	0/7566	0.68	3/10283 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	337	VAL	CB-CA-C	-6.53	99.00	111.40
1	A	37	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	189	ASN	N-CA-CB	-5.60	100.53	110.60

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	3778	0	3579	18	0
1	B	3639	0	3473	35	0
2	A	16	0	11	0	0
2	B	16	0	11	0	0
3	A	56	0	52	0	0
3	B	56	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
4	B	3	0	0	2	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	153	0	0	0	0
7	B	170	0	0	3	0
All	All	7901	0	7178	54	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 4.

All (54) 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:193:GLN:HE22	1:A:297:GLU:H	1.33	0.77
4:B:606:CL:CL	7:B:830:HOH:O	2.42	0.73
1:B:193:GLN:HE22	1:B:297:GLU:H	1.34	0.71
4:B:608:CL:CL	7:B:850:HOH:O	2.48	0.67
1:B:47:LYS:HG2	1:B:47:LYS:O	1.94	0.66
1:B:44:VAL:HG13	1:B:58:VAL:HG13	1.77	0.66
1:B:44:VAL:HG13	1:B:58:VAL:CG1	2.26	0.66
1:B:61:ILE:HG23	1:B:62:ARG:HG3	1.79	0.64
1:A:276:LEU:HD22	1:A:280:ILE:HG12	1.83	0.60
1:B:44:VAL:HG11	1:B:58:VAL:HG11	1.83	0.60
1:B:44:VAL:CG1	1:B:58:VAL:HG11	2.31	0.59
1:B:314:VAL:O	1:B:317:THR:HG23	2.03	0.58
1:A:470:THR:HB	1:A:476:GLN:OE1	2.03	0.58
1:B:111:THR:HG22	1:B:156:LEU:HD13	1.86	0.58
1:A:44:VAL:CG1	1:A:58:VAL:HG11	2.34	0.57
1:A:193:GLN:HE22	1:A:297:GLU:N	2.03	0.56
1:B:470:THR:OG1	1:B:476:GLN:NE2	2.38	0.56
1:B:44:VAL:CG1	1:B:58:VAL:CG1	2.85	0.55
1:B:322:LEU:O	1:B:415:ARG:HD3	2.07	0.54
1:B:193:GLN:HE22	1:B:297:GLU:N	2.03	0.54
1:B:293:TRP:HB2	1:B:317:THR:HB	1.91	0.53
1:B:314:VAL:O	1:B:317:THR:CG2	2.57	0.53
1:B:176:ASN:C	1:B:176:ASN:HD22	2.13	0.52
1:A:326:GLN:HB2	1:A:473:MET:HE1	1.91	0.52
1:B:297:GLU:HB3	7:B:746:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:O	1:A:415:ARG:HD3	2.10	0.50
1:A:44:VAL:HG13	1:A:58:VAL:CG1	2.41	0.50
1:A:314:VAL:HG13	1:A:494:TRP:CE3	2.47	0.49
1:B:283:ILE:HG23	1:B:288:ILE:HB	1.95	0.48
1:B:96:ARG:NH2	1:B:113:SER:OG	2.45	0.48
1:A:283:ILE:HG23	1:A:288:ILE:HB	1.96	0.47
1:B:176:ASN:HD21	1:B:178:ASN:HB2	1.79	0.47
1:A:331:ARG:NH2	1:A:409:ILE:O	2.48	0.47
1:B:203:TYR:OH	1:B:525:GLU:OE2	2.21	0.46
1:B:331:ARG:NH2	1:B:409:ILE:O	2.49	0.46
1:B:314:VAL:HG13	1:B:494:TRP:CE3	2.52	0.45
1:A:117:GLN:HE21	1:A:135:ILE:HB	1.82	0.45
1:A:44:VAL:CG1	1:A:58:VAL:CG1	2.94	0.45
1:A:101:CYS:O	1:A:103:THR:HG23	2.17	0.45
1:A:51:LEU:HD11	1:B:461:LEU:HD13	1.98	0.45
1:B:486:VAL:HG23	3:B:602:NAG:H81	1.99	0.44
1:A:201:ILE:HG23	1:A:206:TRP:HB2	1.98	0.44
1:B:493:ASN:ND2	1:B:495:HIS:HE1	2.14	0.44
1:B:337:VAL:CG2	1:B:408:TYR:OH	2.66	0.43
1:B:201:ILE:HG23	1:B:206:TRP:HB2	2.00	0.43
1:A:44:VAL:HG11	1:A:58:VAL:HG11	2.00	0.43
1:B:525:GLU:H	1:B:525:GLU:CD	2.21	0.43
1:B:493:ASN:HD21	1:B:529:LEU:H	1.66	0.43
1:B:334:LEU:HB3	1:B:409:ILE:CD1	2.50	0.42
1:B:337:VAL:HG22	1:B:408:TYR:OH	2.20	0.42
1:B:187:ILE:CD1	1:B:322:LEU:HD21	2.50	0.41
1:B:472:ASN:HD22	1:B:472:ASN:H	1.69	0.41
1:A:189:ASN:C	1:A:189:ASN:OD1	2.58	0.41
1:B:243:ILE:HD12	1:B:276:LEU:HA	2.02	0.41

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	481/568 (85%)	468 (97%)	13 (3%)	0	100	100
1	B	459/568 (81%)	448 (98%)	11 (2%)	0	100	100
All	All	940/1136 (83%)	916 (97%)	24 (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	390/487 (80%)	369 (95%)	21 (5%)	22	20
1	B	377/487 (77%)	355 (94%)	22 (6%)	20	17
All	All	767/974 (79%)	724 (94%)	43 (6%)	21	18

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	49	GLN
1	A	58	VAL
1	A	108	LEU
1	A	125	LEU
1	A	179	GLN
1	A	189	ASN
1	A	205	ARG
1	A	270	PHE
1	A	276	LEU
1	A	314	VAL
1	A	322	LEU
1	A	323	LYS
1	A	326	GLN
1	A	334	LEU
1	A	455	VAL
1	A	470	THR
1	A	473	MET

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Mol	Chain	Res	Type
1	A	496	LEU
1	A	506	LYS
1	A	537	VAL
1	B	47	LYS
1	B	48	ASP
1	B	56	GLU
1	B	58	VAL
1	B	61	ILE
1	B	117	GLN
1	B	156	LEU
1	B	176	ASN
1	B	179	GLN
1	B	270	PHE
1	B	289	THR
1	B	314	VAL
1	B	317	THR
1	B	322	LEU
1	B	334	LEU
1	B	337	VAL
1	B	357	ASN
1	B	455	VAL
1	B	461	LEU
1	B	472	ASN
1	B	496	LEU
1	B	506	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	117	GLN
1	A	118	ASN
1	A	179	GLN
1	A	193	GLN
1	A	338	HIS
1	A	446	ASN
1	A	493	ASN
1	A	495	HIS
1	B	72	GLN
1	B	118	ASN
1	B	176	ASN
1	B	179	GLN

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Mol	Chain	Res	Type
1	B	193	GLN
1	B	338	HIS
1	B	357	ASN
1	B	472	ASN
1	B	476	GLN
1	B	493	ASN
1	B	495	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	B	482	1	3,6,7	0.44	0	0,6,8	-	-
1	CSO	A	482	1	3,6,7	0.42	0	0,6,8	-	-
1	CSO	B	236	1	3,6,7	0.75	0	0,6,8	-	-
1	CSO	A	236	1	3,6,7	0.68	0	0,6,8	-	-

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
1	CSO	B	482	1	-	0/1/5/7	-
1	CSO	A	482	1	-	0/1/5/7	-
1	CSO	B	236	1	-	0/1/5/7	-
1	CSO	A	236	1	-	0/1/5/7	-

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.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	NAG	A	602	1	14,14,15	0.53	0	17,19,21	2.37	4 (23%)
3	NAG	A	605	1	14,14,15	0.48	0	17,19,21	1.25	1 (5%)
3	NAG	B	605	1	14,14,15	0.69	0	17,19,21	1.30	3 (17%)
3	NAG	A	603	1	14,14,15	0.52	0	17,19,21	1.42	2 (11%)
3	NAG	B	602	1	14,14,15	0.45	0	17,19,21	0.96	1 (5%)
3	NAG	B	603	1	14,14,15	0.63	0	17,19,21	1.36	2 (11%)
5	BCT	B	609	-	2,3,3	0.72	0	2,3,3	0.98	0
3	NAG	A	604	1	14,14,15	0.57	0	17,19,21	1.56	3 (17%)
2	TCR	A	601	-	16,18,18	1.66	2 (12%)	16,26,26	1.38	4 (25%)
3	NAG	B	604	1	14,14,15	0.76	1 (7%)	17,19,21	1.11	1 (5%)
2	TCR	B	601	-	16,18,18	1.89	4 (25%)	16,26,26	1.41	3 (18%)
5	BCT	A	609	-	2,3,3	1.01	0	2,3,3	0.54	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	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	605	1	-	2/6/23/26	0/1/1/1
3	NAG	B	605	1	-	0/6/23/26	0/1/1/1
3	NAG	A	603	1	-	2/6/23/26	0/1/1/1
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1
3	NAG	B	603	1	-	0/6/23/26	0/1/1/1
3	NAG	A	604	1	-	2/6/23/26	0/1/1/1
2	TCR	A	601	-	-	0/4/13/13	0/3/3/3
3	NAG	B	604	1	-	0/6/23/26	0/1/1/1
2	TCR	B	601	-	-	2/4/13/13	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TCR	CG-CD1	4.88	1.46	1.39
2	A	601	TCR	CG-CD1	4.69	1.46	1.39
2	B	601	TCR	CD2-CE2	2.26	1.48	1.42
2	A	601	TCR	CD2-CE2	2.18	1.48	1.42
2	B	601	TCR	CE3-CD2	-2.08	1.38	1.42
2	B	601	TCR	CB-CG	-2.05	1.49	1.51
3	B	604	NAG	C1-C2	2.02	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	NAG	C1-O5-C5	7.54	122.41	112.19
3	A	603	NAG	C1-O5-C5	3.89	117.46	112.19
3	A	605	NAG	C1-O5-C5	3.71	117.22	112.19
3	A	604	NAG	C3-C4-C5	3.38	116.27	110.24
3	A	602	NAG	O5-C5-C4	3.29	118.84	110.83
3	A	604	NAG	O5-C1-C2	-3.24	106.17	111.29
3	A	602	NAG	C3-C4-C5	3.00	115.60	110.24
3	A	603	NAG	O5-C5-C6	2.76	111.54	107.20
3	B	603	NAG	C1-O5-C5	2.69	115.84	112.19
2	B	601	TCR	CE3-CD2-CE2	2.65	121.69	118.17
2	B	601	TCR	CB-CA-C	-2.54	106.17	112.06
3	B	605	NAG	O5-C5-C6	2.50	111.13	107.20
2	A	601	TCR	CE3-CD2-CE2	2.47	121.44	118.17
3	B	602	NAG	O5-C1-C2	-2.44	107.44	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	605	NAG	O5-C5-C4	-2.38	105.04	110.83
2	B	601	TCR	CZ3-CE3-CD2	-2.34	117.65	120.89
3	B	605	NAG	C3-C4-C5	-2.34	106.07	110.24
3	B	603	NAG	O3-C3-C4	-2.30	105.02	110.35
3	B	604	NAG	O5-C5-C6	2.22	110.68	107.20
2	A	601	TCR	CZ3-CE3-CD2	-2.20	117.85	120.89
2	A	601	TCR	C-CA-N	-2.12	105.80	108.97
2	A	601	TCR	OXT-C-CA	2.09	120.36	113.40
3	A	604	NAG	C4-C3-C2	2.01	113.97	111.02
3	A	602	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	605	NAG	O5-C5-C6-O6
3	A	603	NAG	O5-C5-C6-O6
3	A	604	NAG	C4-C5-C6-O6
3	A	603	NAG	C4-C5-C6-O6
2	B	601	TCR	OXT-C-CA-N
3	A	605	NAG	C4-C5-C6-O6
3	A	604	NAG	C3-C2-N2-C7
2	B	601	TCR	O1-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	NAG	1	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	485/568 (85%)	0.44	46 (9%)	8	10	25, 45, 86, 109	0
1	B	465/568 (81%)	0.20	27 (5%)	23	28	23, 40, 68, 89	0
All	All	950/1136 (83%)	0.32	73 (7%)	13	17	23, 42, 77, 109	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	HIS	5.9
1	B	48	ASP	5.7
1	B	46	ALA	5.3
1	A	131	CYS	5.2
1	A	129	CYS	5.0
1	B	47	LYS	4.8
1	A	135	ILE	4.5
1	A	120	ILE	4.5
1	A	46	ALA	4.4
1	A	132	SER	4.3
1	A	533	PHE	4.3
1	A	124	ASN	4.2
1	A	398	ASP	4.2
1	A	126	ASP	4.1
1	A	395	CYS	4.1
1	A	128	PHE	4.1
1	A	136	PRO	4.0
1	A	396	THR	3.9
1	B	360	LEU	3.8
1	A	446	ASN	3.8
1	B	396	THR	3.8
1	B	395	CYS	3.5
1	B	21	GLY	3.5
1	B	121	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	127	GLU	3.3
1	A	404	VAL	3.2
1	A	445	THR	3.2
1	A	23	ASP	3.2
1	A	133	GLU	3.1
1	A	130	ASN	3.0
1	B	404	VAL	2.9
1	A	453	LYS	2.9
1	A	444	PHE	2.9
1	A	22	PRO	2.9
1	A	125	LEU	2.8
1	A	394	LEU	2.8
1	A	86	ALA	2.7
1	B	119	LYS	2.7
1	B	394	LEU	2.7
1	A	498	PRO	2.7
1	B	85	PRO	2.7
1	A	442	GLY	2.7
1	B	86	ALA	2.7
1	B	398	ASP	2.7
1	B	120	ILE	2.6
1	A	393	PRO	2.6
1	B	149	VAL	2.5
1	B	37	LEU	2.5
1	A	497	SER	2.4
1	A	499	GLU	2.4
1	B	498	PRO	2.4
1	A	435	TYR	2.3
1	A	403	SER	2.3
1	B	397	GLY	2.3
1	A	122	SER	2.3
1	B	401	ILE	2.3
1	B	117	GLN	2.2
1	A	123	LEU	2.2
1	A	253	GLN	2.2
1	B	253	GLN	2.2
1	A	144	ALA	2.2
1	A	510	TYR	2.2
1	A	400	ASN	2.1
1	A	496	LEU	2.1
1	B	142	VAL	2.1
1	B	518	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	399	GLU	2.1
1	A	352	TRP	2.1
1	B	153	VAL	2.1
1	B	144	ALA	2.1
1	A	298	ALA	2.0
1	B	141	VAL	2.0
1	A	358	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
1	CSO	B	236	7/8	0.89	0.10	37,38,49,53	0
1	CSO	A	236	7/8	0.93	0.10	37,37,44,49	0
1	CSO	B	482	7/8	0.93	0.10	35,37,54,56	0
1	CSO	A	482	7/8	0.96	0.08	32,35,45,53	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	NAG	B	604	14/15	0.42	0.36	91,101,104,106	0
3	NAG	A	604	14/15	0.71	0.33	75,88,92,92	0
3	NAG	B	605	14/15	0.74	0.41	74,86,100,107	0
3	NAG	A	602	14/15	0.79	0.20	62,66,73,76	0
3	NAG	A	605	14/15	0.86	0.38	62,75,86,86	0
3	NAG	A	603	14/15	0.88	0.22	79,82,87,87	0
4	CL	A	608	1/1	0.90	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	B	602	14/15	0.91	0.21	47,60,65,67	0
3	NAG	B	603	14/15	0.94	0.10	46,48,54,54	0
6	MG	A	610	1/1	0.94	0.07	56,56,56,56	0
5	BCT	B	609	4/4	0.96	0.11	28,33,35,38	0
2	TCR	B	601	16/16	0.96	0.15	23,35,43,46	0
2	TCR	A	601	16/16	0.97	0.16	25,33,39,40	0
4	CL	B	608	1/1	0.97	0.06	58,58,58,58	0
6	MG	B	611	1/1	0.97	0.19	57,57,57,57	0
5	BCT	A	609	4/4	0.98	0.12	34,36,36,40	0
4	CL	B	606	1/1	0.98	0.10	43,43,43,43	0
4	CL	B	607	1/1	0.99	0.17	49,49,49,49	0
4	CL	A	606	1/1	0.99	0.13	42,42,42,42	0
6	MG	B	610	1/1	0.99	0.05	45,45,45,45	0
4	CL	A	607	1/1	0.99	0.15	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.