Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 10:33 AM EDT

PDB ID	:	5FBH
Title	:	Crystal structure of the extracellular domain of human calcium sensing receptor with bound Gd3+
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	:	2.70 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:

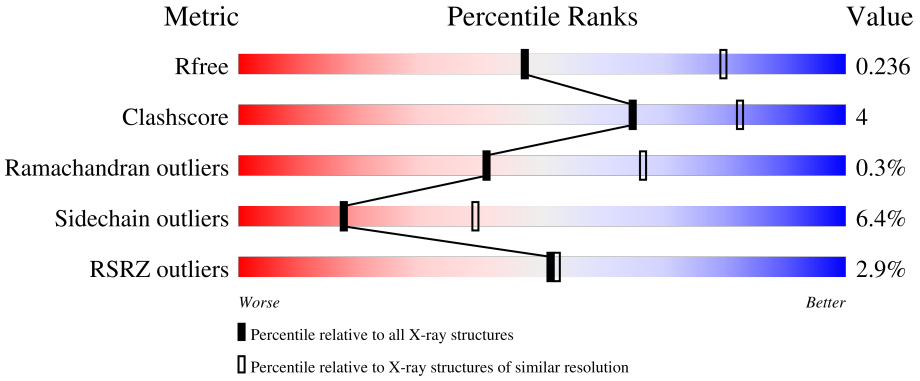
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	4% 71% 10% • 17%
1	B	568	% 73% 9% • 17%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7394 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	B	470	3628	2328	615	673	12	0	0	0
1	A	472	3604	2312	607	673	12	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

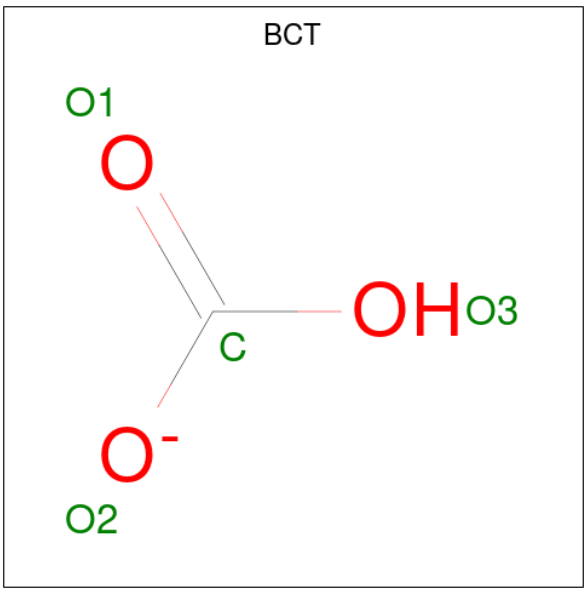
- Molecule 2 is GADOLINIUM ION (three-letter code: GD3) (formula: Gd).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

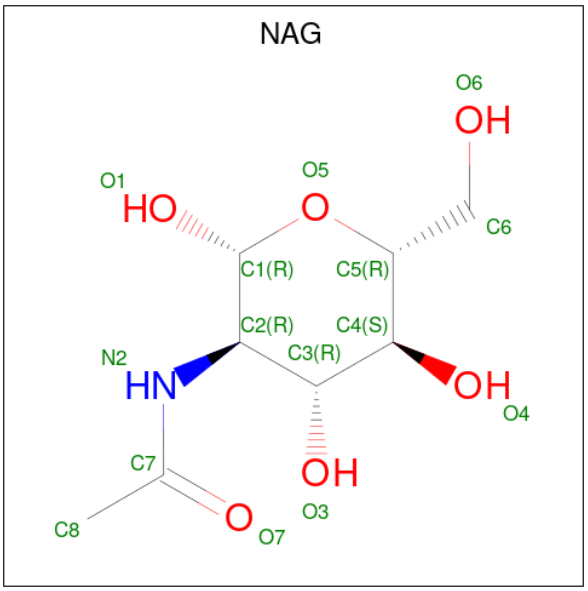


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	4	1	3	0	0
			Total	C	O		
4	A	1	4	1	3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

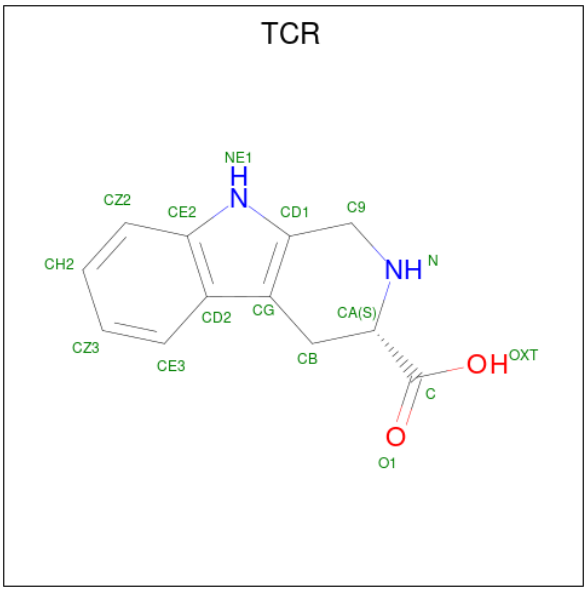
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	B	1	1	1	0	0
			Total	Cl		
5	A	1	1	1	0	0

- Molecule 6 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		
6	B	1	14	8	1	5	0	0
			Total	C	N	O		
6	B	1	14	8	1	5	0	0
			Total	C	N	O		
6	B	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0

- Molecule 7 is CYCLOMETHYLTRYPTOPHAN (three-letter code: TCR) (formula: $C_{12}H_{12}N_2O_2$).



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

- Molecule 8 is water.

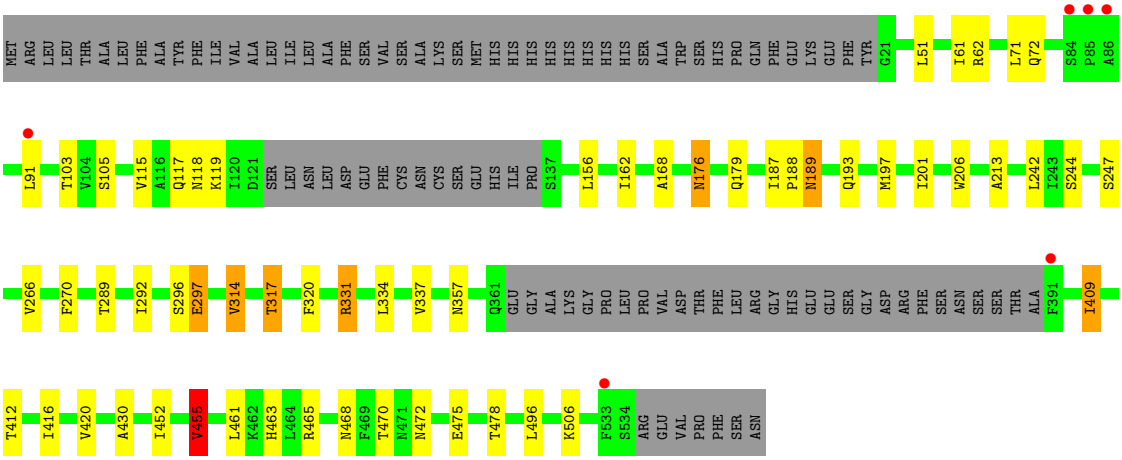
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	B	11	11	11	0	0
			Total	O		
8	A	6	6	6	0	0

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.

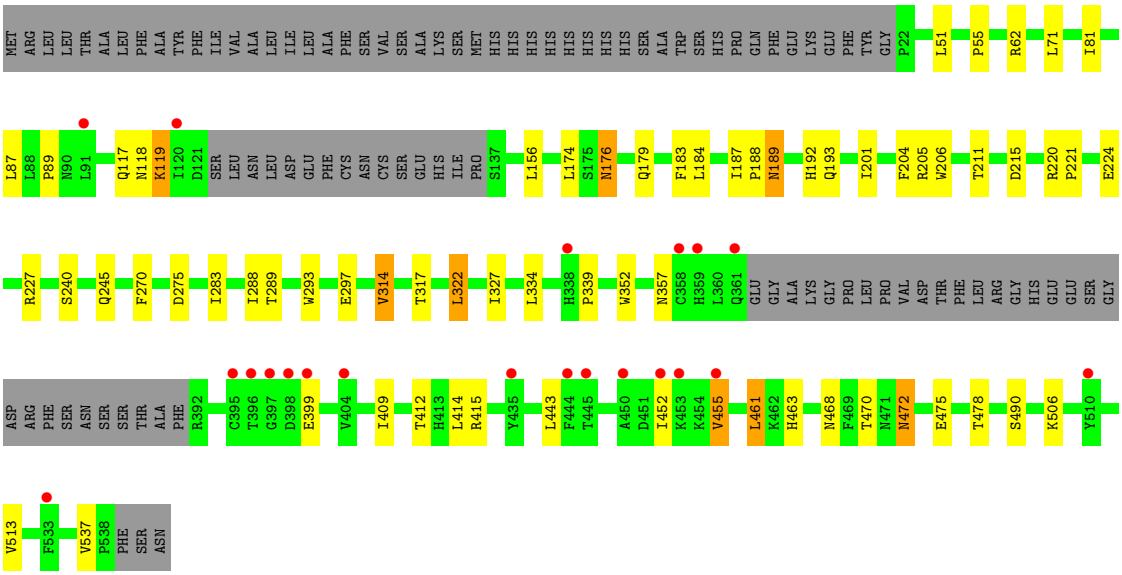
• Molecule 1: Extracellular calcium-sensing receptor

Chain B:



• Molecule 1: Extracellular calcium-sensing receptor

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	172.11Å 83.11Å 94.47Å 90.00° 105.15° 90.00°	Depositor
Resolution (Å)	46.08 – 2.70 46.08 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (46.08-2.70) 97.4 (46.08-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.182 , 0.236 0.188 , 0.236	Depositor DCC
R_{free} test set	1733 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7394	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: CSO, NAG, GD3, CL, TCR, BCT, MG

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	0.58	0/3676	0.73	1/5007 (0.0%)
1	B	0.65	0/3701	0.78	2/5031 (0.0%)
All	All	0.62	0/7377	0.76	3/10038 (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	A	537	VAL	C-N-CA	6.91	151.00	122.00
1	B	455	VAL	CB-CA-C	-5.57	100.82	111.40
1	B	331	ARG	NE-CZ-NH1	5.01	122.80	120.30

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	3604	0	3360	32	0
1	B	3628	0	3437	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	0	1	0
4	B	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	56	0	52	0	0
6	B	42	0	39	0	0
7	A	16	0	11	0	0
7	B	16	0	11	1	0
8	A	6	0	0	0	0
8	B	11	0	0	0	0
All	All	7394	0	6910	58	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 (58) 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:314:VAL:O	1:A:317:THR:HG23	1.80	0.81
1:B:314:VAL:O	1:B:317:THR:HG23	1.86	0.76
1:A:71:LEU:C	1:A:71:LEU:HD23	2.15	0.67
1:A:193:GLN:HE22	1:A:297:GLU:H	1.48	0.62
1:B:468:ASN:HA	1:B:478:THR:HG22	1.84	0.59
1:B:197:MET:HG3	1:B:320:PHE:HE2	1.67	0.59
1:B:452:ILE:HA	1:B:455:VAL:HG22	1.86	0.58
1:B:72:GLN:HA	1:B:72:GLN:HE21	1.72	0.54
1:B:197:MET:HG3	1:B:320:PHE:CE2	2.42	0.54
1:B:176:ASN:C	1:B:176:ASN:HD22	2.11	0.54
1:A:189:ASN:C	1:A:189:ASN:OD1	2.47	0.53
1:A:176:ASN:C	1:A:176:ASN:HD22	2.11	0.53
1:B:314:VAL:O	1:B:317:THR:CG2	2.57	0.52
1:A:314:VAL:O	1:A:317:THR:CG2	2.56	0.51
1:B:168:ALA:O	7:B:609:TCR:H91	2.10	0.51
1:B:71:LEU:C	1:B:71:LEU:HD23	2.31	0.51
1:B:193:GLN:HE22	1:B:296:SER:HA	1.76	0.50
1:A:192:HIS:NE2	1:A:513:VAL:HG13	2.27	0.50
1:A:443:LEU:HD12	1:A:463:HIS:CE1	2.47	0.49
1:B:51:LEU:HD11	1:A:461:LEU:HD13	1.95	0.49
1:B:189:ASN:OD1	1:B:189:ASN:C	2.50	0.49
1:B:193:GLN:HE22	1:B:297:GLU:H	1.62	0.48
1:A:176:ASN:C	1:A:176:ASN:ND2	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HD3	1:A:119:LYS:HE2	1.96	0.48
1:B:193:GLN:NE2	1:B:296:SER:HA	2.29	0.47
1:A:204:PHE:C	1:A:205:ARG:HG2	2.36	0.47
1:A:452:ILE:HA	1:A:455:VAL:HG22	1.97	0.46
1:A:472:ASN:HD22	1:A:472:ASN:H	1.63	0.46
1:B:266:VAL:HG22	1:B:292:ILE:HB	1.98	0.46
1:A:201:ILE:HG23	1:A:206:TRP:HB2	1.96	0.46
1:A:470:THR:HA	1:A:475:GLU:O	2.16	0.46
1:A:415:ARG:N	4:A:603:BCT:O1	2.42	0.45
1:A:211:THR:O	1:A:240:SER:HA	2.16	0.45
1:B:213:ALA:O	1:B:242:LEU:HA	2.18	0.44
1:A:322:LEU:O	1:A:415:ARG:HD3	2.18	0.43
1:B:61:ILE:HG23	1:B:62:ARG:HG3	1.99	0.43
1:A:220:ARG:HB2	1:A:221:PRO:HD3	2.01	0.43
1:B:115:VAL:HG12	1:B:162:ILE:HD12	2.00	0.43
1:A:118:ASN:ND2	1:A:118:ASN:H	2.18	0.42
1:B:201:ILE:HG23	1:B:206:TRP:HB2	2.01	0.42
1:B:430:ALA:HB1	1:B:463:HIS:HB3	2.02	0.42
1:B:470:THR:HA	1:B:475:GLU:O	2.18	0.42
1:A:51:LEU:CD2	1:A:55:PRO:HG3	2.50	0.42
1:A:283:ILE:HG23	1:A:288:ILE:HB	2.02	0.42
1:B:187:ILE:HG13	1:B:188:PRO:HD2	2.01	0.41
1:B:416:ILE:O	1:B:420:VAL:HG23	2.20	0.41
1:A:327:ILE:HD12	1:A:414:LEU:HD13	2.02	0.41
1:A:468:ASN:HA	1:A:478:THR:HG22	2.02	0.41
1:B:331:ARG:NH2	1:B:409:ILE:O	2.54	0.41
1:B:103:THR:HG22	1:B:105:SER:H	1.86	0.41
1:A:174:LEU:HB3	1:A:183:PHE:CE1	2.56	0.41
1:A:245:GLN:N	1:A:275:ASP:HA	2.36	0.41
1:B:193:GLN:HE22	1:B:296:SER:CA	2.33	0.40
1:A:215:ASP:OD1	1:A:220:ARG:HD3	2.21	0.40
1:A:81:ILE:HG23	1:A:87:LEU:HD23	2.03	0.40
1:A:339:PRO:HD3	1:A:352:TRP:CE3	2.56	0.40
1:A:187:ILE:HG13	1:A:188:PRO:HD2	2.03	0.40
1:A:293:TRP:HB2	1:A:317:THR:HG22	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	464/568 (82%)	436 (94%)	26 (6%)	2 (0%)	34	60
1	B	462/568 (81%)	440 (95%)	21 (4%)	1 (0%)	47	73
All	All	926/1136 (82%)	876 (95%)	47 (5%)	3 (0%)	41	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	118	ASN
1	A	62	ARG
1	A	89	PRO

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	362/487 (74%)	339 (94%)	23 (6%)	17	39
1	B	370/487 (76%)	346 (94%)	24 (6%)	17	38
All	All	732/974 (75%)	685 (94%)	47 (6%)	17	39

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	91	LEU
1	B	117	GLN
1	B	156	LEU

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Mol	Chain	Res	Type
1	B	176	ASN
1	B	179	GLN
1	B	189	ASN
1	B	244	SER
1	B	247	SER
1	B	270	PHE
1	B	289	THR
1	B	297	GLU
1	B	314	VAL
1	B	317	THR
1	B	334	LEU
1	B	337	VAL
1	B	357	ASN
1	B	409	ILE
1	B	412	THR
1	B	455	VAL
1	B	461	LEU
1	B	465	ARG
1	B	472	ASN
1	B	496	LEU
1	B	506	LYS
1	A	117	GLN
1	A	119	LYS
1	A	156	LEU
1	A	176	ASN
1	A	179	GLN
1	A	184	LEU
1	A	189	ASN
1	A	224	GLU
1	A	227	ARG
1	A	270	PHE
1	A	289	THR
1	A	314	VAL
1	A	322	LEU
1	A	334	LEU
1	A	357	ASN
1	A	399	GLU
1	A	409	ILE
1	A	412	THR
1	A	455	VAL
1	A	461	LEU
1	A	472	ASN

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Mol	Chain	Res	Type
1	A	490	SER
1	A	506	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	GLN
1	B	118	ASN
1	B	176	ASN
1	B	179	GLN
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
1	B	524	ASN
1	A	72	GLN
1	A	118	ASN
1	A	176	ASN
1	A	179	GLN
1	A	193	GLN
1	A	413	HIS
1	A	463	HIS
1	A	472	ASN
1	A	493	ASN
1	A	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	A	236	1	3,6,7	0.69	0	0,6,8	-	-
1	CSO	B	236	1	3,6,7	0.56	0	0,6,8	-	-
1	CSO	A	482	1	3,6,7	0.62	0	0,6,8	-	-
1	CSO	B	482	1	3,6,7	0.39	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	A	236	1	-	0/1/5/7	-
1	CSO	B	236	1	-	0/1/5/7	-
1	CSO	A	482	1	-	0/1/5/7	-
1	CSO	B	482	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 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
6	NAG	B	607	1	14,14,15	0.58	0	17,19,21	0.95	1 (5%)
6	NAG	B	608	1	14,14,15	0.54	0	17,19,21	2.18	7 (41%)
6	NAG	A	606	1	14,14,15	0.63	0	17,19,21	1.59	3 (17%)
4	BCT	A	603	-	2,3,3	0.53	0	2,3,3	2.97	2 (100%)
4	BCT	B	604	-	2,3,3	0.78	0	2,3,3	0.68	0
6	NAG	A	608	1	14,14,15	0.56	0	17,19,21	2.11	6 (35%)
6	NAG	A	605	1	14,14,15	0.58	0	17,19,21	1.26	1 (5%)
7	TCR	B	609	-	16,18,18	1.85	2 (12%)	16,26,26	1.95	4 (25%)
7	TCR	A	609	-	16,18,18	2.62	6 (37%)	16,26,26	2.38	3 (18%)
6	NAG	B	606	1	14,14,15	0.52	0	17,19,21	2.20	4 (23%)
6	NAG	A	607	1	14,14,15	0.53	0	17,19,21	1.55	5 (29%)

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
6	NAG	B	607	1	-	2/6/23/26	0/1/1/1
6	NAG	B	608	1	-	2/6/23/26	0/1/1/1
6	NAG	A	606	1	-	1/6/23/26	0/1/1/1
6	NAG	A	608	1	-	4/6/23/26	0/1/1/1
6	NAG	A	605	1	-	2/6/23/26	0/1/1/1
7	TCR	B	609	-	-	0/4/13/13	0/3/3/3
7	TCR	A	609	-	-	0/4/13/13	0/3/3/3
6	NAG	B	606	1	-	2/6/23/26	0/1/1/1
6	NAG	A	607	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	609	TCR	CG-CD1	6.88	1.49	1.39
7	A	609	TCR	CB-CG	-4.36	1.46	1.51
7	B	609	TCR	CG-CD1	4.28	1.45	1.39
7	A	609	TCR	CZ2-CE2	-2.83	1.37	1.41
7	A	609	TCR	CD2-CE2	2.63	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	609	TCR	CE3-CD2	-2.51	1.37	1.42
7	B	609	TCR	CB-CG	-2.33	1.48	1.51
7	A	609	TCR	O1-C	2.18	1.28	1.22

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	609	TCR	CB-CA-N	7.53	128.06	112.50
6	B	606	NAG	C1-O5-C5	7.41	122.24	112.19
6	A	608	NAG	C1-O5-C5	5.16	119.19	112.19
6	B	608	NAG	O5-C5-C6	4.64	114.48	107.20
6	A	605	NAG	C1-O5-C5	3.94	117.53	112.19
6	A	608	NAG	C8-C7-N2	3.93	122.75	116.10
6	B	608	NAG	O3-C3-C2	3.76	117.25	109.47
7	B	609	TCR	CE3-CD2-CE2	3.71	123.08	118.17
4	A	603	BCT	O3-C-O1	-3.47	110.54	119.55
6	A	606	NAG	C3-C4-C5	3.43	116.36	110.24
6	A	606	NAG	O5-C1-C2	-3.41	105.90	111.29
7	A	609	TCR	CZ3-CE3-CD2	-3.37	116.22	120.89
7	B	609	TCR	CB-CA-C	-3.34	104.32	112.06
6	B	608	NAG	C6-C5-C4	-3.16	105.61	113.00
7	B	609	TCR	CZ3-CE3-CD2	-3.12	116.57	120.89
7	A	609	TCR	CE3-CD2-CE2	3.03	122.18	118.17
6	A	608	NAG	C4-C3-C2	-2.94	106.71	111.02
6	B	608	NAG	O7-C7-C8	-2.94	116.60	122.06
6	A	607	NAG	O5-C5-C6	2.89	111.73	107.20
6	A	608	NAG	O7-C7-C8	-2.88	116.70	122.06
6	B	606	NAG	C1-C2-N2	2.83	115.32	110.49
6	A	607	NAG	C1-O5-C5	2.79	115.97	112.19
6	B	607	NAG	O5-C5-C6	2.49	111.10	107.20
6	A	608	NAG	C1-C2-N2	2.46	114.69	110.49
6	A	608	NAG	C2-N2-C7	2.43	126.36	122.90
6	B	608	NAG	C1-C2-N2	2.41	114.61	110.49
4	A	603	BCT	O2-C-O1	2.35	125.64	119.55
6	A	606	NAG	C1-C2-N2	2.34	114.49	110.49
7	B	609	TCR	C-CA-N	-2.33	105.50	108.97
6	B	608	NAG	C1-O5-C5	2.23	115.21	112.19
6	B	606	NAG	O7-C7-C8	-2.21	117.95	122.06
6	A	607	NAG	C6-C5-C4	-2.09	108.11	113.00
6	A	607	NAG	C3-C4-C5	2.06	113.91	110.24
6	A	607	NAG	C1-C2-N2	2.05	113.98	110.49
6	B	608	NAG	O4-C4-C3	-2.00	105.72	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	606	NAG	O7-C7-N2	2.00	125.63	121.95

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	607	NAG	O5-C5-C6-O6
6	B	606	NAG	O5-C5-C6-O6
6	A	608	NAG	O5-C5-C6-O6
6	B	607	NAG	C4-C5-C6-O6
6	A	608	NAG	C8-C7-N2-C2
6	A	608	NAG	O7-C7-N2-C2
6	A	608	NAG	C4-C5-C6-O6
6	B	606	NAG	C4-C5-C6-O6
6	A	607	NAG	O5-C5-C6-O6
6	B	608	NAG	O5-C5-C6-O6
6	A	605	NAG	C4-C5-C6-O6
6	A	606	NAG	C4-C5-C6-O6
6	A	605	NAG	O5-C5-C6-O6
6	A	607	NAG	C4-C5-C6-O6
6	B	608	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	BCT	1	0
7	B	609	TCR	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	470/568 (82%)	0.10	21 (4%)	33	31	40, 67, 110, 144	0
1	B	468/568 (82%)	0.02	6 (1%)	77	78	38, 60, 98, 126	0
All	All	938/1136 (82%)	0.06	27 (2%)	51	52	38, 63, 105, 144	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	LEU	4.8
1	A	404	VAL	4.5
1	A	435	TYR	4.4
1	A	359	HIS	3.7
1	A	361	GLN	3.7
1	A	533	PHE	3.5
1	A	358	CYS	3.5
1	A	396	THR	3.2
1	A	398	ASP	3.1
1	A	395	CYS	3.1
1	A	120	ILE	2.9
1	B	84	SER	2.8
1	A	445	THR	2.7
1	A	397	GLY	2.7
1	B	391	PHE	2.7
1	A	338	HIS	2.6
1	A	444	PHE	2.4
1	A	455	VAL	2.3
1	B	85	PRO	2.3
1	B	533	PHE	2.2
1	A	453	LYS	2.2
1	A	450	ALA	2.2
1	A	452	ILE	2.1
1	A	510	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	91	LEU	2.1
1	A	399	GLU	2.1
1	B	86	ALA	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	0.92	0.20	53,57,78,78	0
1	CSO	A	236	7/8	0.94	0.13	48,52,65,77	0
1	CSO	A	482	7/8	0.94	0.14	58,60,67,82	0
1	CSO	B	482	7/8	0.97	0.10	54,65,80,80	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
6	NAG	A	606	14/15	0.84	0.42	93,124,141,144	0
6	NAG	B	606	14/15	0.86	0.29	88,112,125,126	0
6	NAG	A	605	14/15	0.88	0.37	95,105,120,121	0
3	MG	A	602	1/1	0.88	0.26	95,95,95,95	0
6	NAG	B	607	14/15	0.89	0.31	109,121,131,133	0
6	NAG	A	608	14/15	0.90	0.26	96,106,121,134	0
5	CL	A	604	1/1	0.92	0.17	65,65,65,65	0
3	MG	B	603	1/1	0.92	0.38	77,77,77,77	0
5	CL	B	605	1/1	0.92	0.24	71,71,71,71	0
6	NAG	A	607	14/15	0.93	0.30	89,109,114,114	0
3	MG	B	602	1/1	0.93	0.37	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	B	608	14/15	0.95	0.20	59,62,79,81	0
7	TCR	A	609	16/16	0.96	0.15	32,42,50,55	0
2	GD3	A	601	1/1	0.97	0.07	120,120,120,120	0
7	TCR	B	609	16/16	0.97	0.17	31,47,58,63	0
4	BCT	A	603	4/4	0.97	0.11	61,61,67,70	0
4	BCT	B	604	4/4	0.99	0.15	45,56,57,64	0
2	GD3	B	601	1/1	1.00	0.10	107,107,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.