



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2016 – 08:03 PM 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

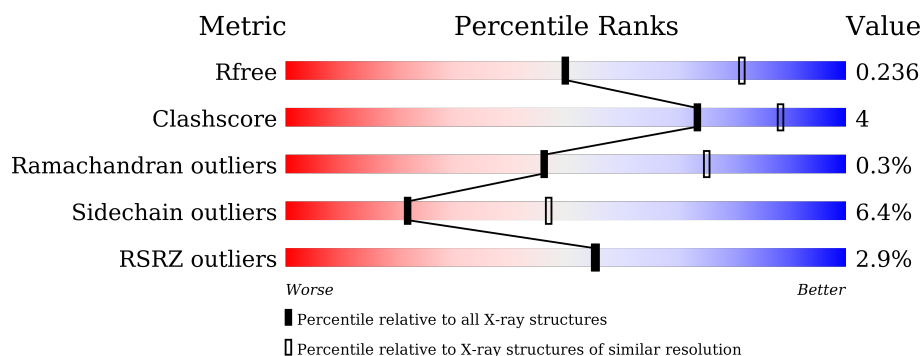
1 Overall quality at a glance

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 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 $\leq 5\%$. 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	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>10%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	568	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>9%</div> <div>•</div> <div>17%</div> </div> </div>

2 Entry composition

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
1	B	470	Total	C	N	O	S	0	0	0
			3628	2328	615	673	12			
1	A	472	Total	C	N	O	S	0	0	0
			3604	2312	607	673	12			

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

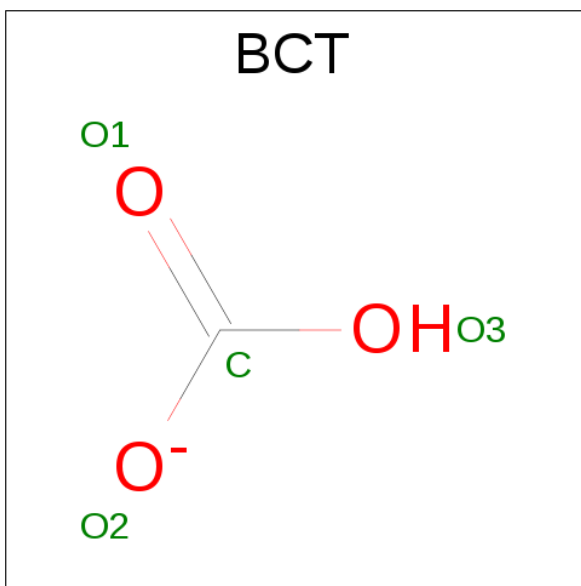
- Molecule 2 is GADOLINIUM ION (three-letter code: GD3) (formula: Gd).

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).

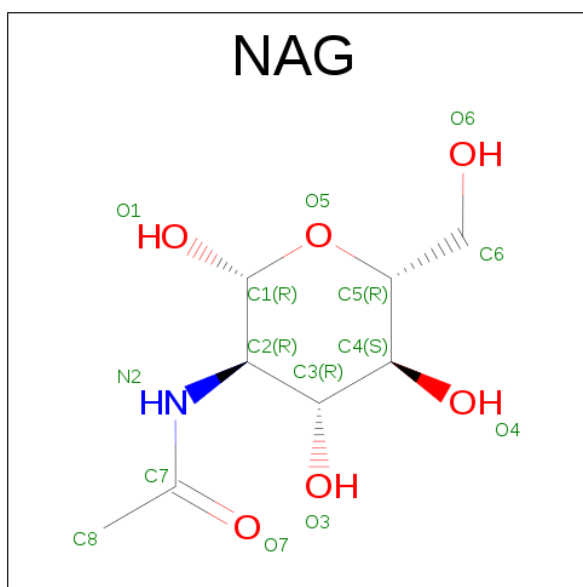


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	1	3		
4	A	1	Total	C	O	0	0
			4	1	3		

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

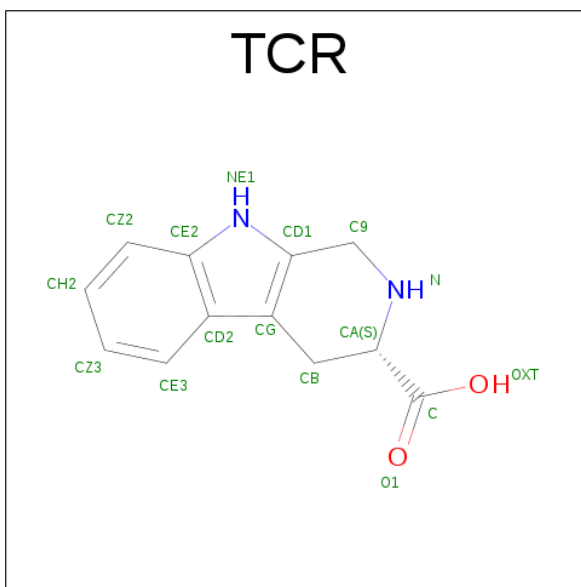
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



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

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



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

- Molecule 8 is water.

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

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	1731 reflections (5.24%)	DCC
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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, GD3, NAG, CL, TCR, CSO, BCT

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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

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:HD23	1:A:71:LEU:C	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:HD22	1:B:176:ASN:C	2.11	0.54
1:A:189:ASN:OD1	1:A:189:ASN:C	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:HD23	1:B:71:LEU:C	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:189:ASN:C	1:B:189:ASN:OD1	2.50	0.49
1:B:51:LEU:HD11	1:A:461:LEU:HD13	1.95	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

Continued on next page...

Continued from previous page...

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:H	1:A:472:ASN:HD22	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:A:220:ARG:HB2	1:A:221:PRO:HD3	2.01	0.43
1:B:61:ILE:HG23	1:B:62:ARG:HG3	1.99	0.43
1:B:115:VAL:HG12	1:B:162:ILE:HD12	2.00	0.43
1:A:118:ASN:H	1:A:118:ASN:ND2	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:283:ILE:HG23	1:A:288:ILE:HB	2.02	0.42
1:A:51:LEU:CD2	1:A:55:PRO:HG3	2.50	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:A:215:ASP:OD1	1:A:220:ARG:HD3	2.21	0.40
1:B:193:GLN:HE22	1:B:296:SER:CA	2.33	0.40
1:A:339:PRO:HD3	1:A:352:TRP:CE3	2.56	0.40
1:A:81:ILE:HG23	1:A:87:LEU:HD23	2.03	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

5.3.1 Protein backbone

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%)	39	69
1	B	462/568 (81%)	440 (95%)	21 (4%)	1 (0%)	52	80
All	All	926/1136 (82%)	876 (95%)	47 (5%)	3 (0%)	46	75

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

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%)	22	47
1	B	370/487 (76%)	346 (94%)	24 (6%)	21	46
All	All	732/974 (75%)	685 (94%)	47 (6%)	22	47

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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	1.86	1 (33%)	2,6,8	1.38	0
1	CSO	A	482	1	3,6,7	2.40	1 (33%)	2,6,8	1.54	0
1	CSO	B	236	1	3,6,7	1.53	1 (33%)	2,6,8	1.67	0
1	CSO	B	482	1	3,6,7	1.84	1 (33%)	2,6,8	2.00	2 (100%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	482	CSO	CB-SG	-4.05	1.76	1.82
1	A	236	CSO	CB-SG	-3.14	1.77	1.82
1	B	482	CSO	CB-SG	-3.12	1.78	1.82
1	B	236	CSO	CB-SG	-2.52	1.78	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	482	CSO	O-C-CA	-2.01	120.34	125.72
1	B	482	CSO	CA-CB-SG	-2.00	107.12	114.09

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 carbohydrates 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	$\# Z > 2$
4	BCT	A	603	-	0,3,3	0.00	-	0,3,3	0.00	-
6	NAG	A	605	1	14,14,15	0.56	0	15,19,21	1.25	1 (6%)
6	NAG	A	606	1	14,14,15	0.60	0	15,19,21	1.44	2 (13%)
6	NAG	A	607	1	14,14,15	0.52	0	15,19,21	1.38	3 (20%)
6	NAG	A	608	1	14,14,15	0.54	0	15,19,21	2.03	5 (33%)
7	TCR	A	609	-	12,18,18	2.41	6 (50%)	10,26,26	1.43	1 (10%)
4	BCT	B	604	-	0,3,3	0.00	-	0,3,3	0.00	-
6	NAG	B	606	1	14,14,15	0.49	0	15,19,21	2.12	3 (20%)
6	NAG	B	607	1	14,14,15	0.55	0	15,19,21	0.77	0
6	NAG	B	608	1	14,14,15	0.52	0	15,19,21	2.06	6 (40%)
7	TCR	B	609	-	12,18,18	1.77	1 (8%)	10,26,26	1.86	2 (20%)

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
4	BCT	A	603	-	-	0/0/0/0	0/0/0/0
6	NAG	A	605	1	-	0/6/23/26	0/1/1/1
6	NAG	A	606	1	-	0/6/23/26	0/1/1/1
6	NAG	A	607	1	-	0/6/23/26	0/1/1/1
6	NAG	A	608	1	-	0/6/23/26	0/1/1/1
7	TCR	A	609	-	-	0/0/13/13	0/3/3/3
4	BCT	B	604	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	606	1	-	0/6/23/26	0/1/1/1
6	NAG	B	607	1	-	0/6/23/26	0/1/1/1
6	NAG	B	608	1	-	0/6/23/26	0/1/1/1
7	TCR	B	609	-	-	0/0/13/13	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	609	TCR	CZ2-CE2	-2.70	1.37	1.41
7	A	609	TCR	CE3-CD2	-2.52	1.37	1.42
7	A	609	TCR	C9-N	-2.07	1.44	1.46
7	A	609	TCR	CD2-CE2	2.63	1.49	1.42
7	A	609	TCR	CG-CD2	2.64	1.46	1.41
7	B	609	TCR	CG-CD1	3.29	1.45	1.39
7	A	609	TCR	CG-CD1	5.27	1.49	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	609	TCR	CB-CA-C	-3.90	104.32	111.48
7	A	609	TCR	CZ3-CE3-CD2	-3.36	116.22	120.88
7	B	609	TCR	CZ3-CE3-CD2	-3.11	116.57	120.88
6	A	608	NAG	C4-C3-C2	-2.98	106.71	111.34
6	B	608	NAG	O7-C7-C8	-2.97	116.60	122.07
6	B	608	NAG	C6-C5-C4	-2.94	105.61	112.99
6	A	608	NAG	O7-C7-C8	-2.92	116.70	122.07
6	B	606	NAG	O7-C7-C8	-2.24	117.95	122.07
6	B	608	NAG	O4-C4-C3	-2.06	105.72	110.36
6	A	607	NAG	O5-C5-C6	2.05	111.73	107.34
6	A	607	NAG	C3-C4-C5	2.06	113.91	110.23
6	B	608	NAG	C1-O5-C5	2.09	115.21	112.14
6	B	606	NAG	O5-C5-C4	2.20	113.78	110.13
6	A	608	NAG	C2-N2-C7	2.50	126.36	123.11
6	A	607	NAG	C1-O5-C5	2.61	115.97	112.14
6	A	606	NAG	O5-C5-C4	3.08	115.24	110.13
6	B	608	NAG	O5-C5-C6	3.33	114.48	107.34
6	A	606	NAG	C3-C4-C5	3.44	116.36	110.23
6	A	608	NAG	C8-C7-N2	3.47	122.75	116.10
6	A	605	NAG	C1-O5-C5	3.66	117.53	112.14
6	B	608	NAG	O3-C3-C2	3.68	117.25	109.37
6	A	608	NAG	C1-O5-C5	4.79	119.19	112.14
6	B	606	NAG	C1-O5-C5	6.87	122.24	112.14

There are no chirality outliers.

There are no torsion outliers.

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

6.1 Protein, DNA and RNA chains

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%) 37 36	40, 67, 110, 144	0
1	B	468/568 (82%)	0.02	6 (1%) 79 79	38, 60, 98, 126	0
All	All	938/1136 (82%)	0.06	27 (2%) 55 55	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	397	GLY	2.7
1	A	445	THR	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	91	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	510	TYR	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. 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
1	CSO	A	482	7/8	0.94	0.14	-	58,60,67,82	0
1	CSO	A	236	7/8	0.94	0.13	-	48,52,65,77	0
1	CSO	B	236	7/8	0.92	0.20	-	53,57,78,78	0
1	CSO	B	482	7/8	0.97	0.10	-	54,65,80,80	0

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
5	CL	B	605	1/1	0.92	0.24	1.17	71,71,71,71	0
6	NAG	A	608	14/15	0.90	0.26	0.98	96,106,121,134	0
3	MG	B	603	1/1	0.92	0.38	0.71	77,77,77,77	0
3	MG	A	602	1/1	0.88	0.26	0.70	95,95,95,95	0
6	NAG	B	608	14/15	0.95	0.20	0.66	59,62,79,81	0
5	CL	A	604	1/1	0.92	0.17	-0.39	65,65,65,65	0
7	TCR	A	609	16/16	0.96	0.15	-1.20	32,42,50,55	0
7	TCR	B	609	16/16	0.97	0.17	-1.92	31,47,58,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BCT	B	604	4/4	0.99	0.15	-2.06	45,56,57,64	0
4	BCT	A	603	4/4	0.97	0.11	-2.18	61,61,67,70	0
6	NAG	A	605	14/15	0.88	0.37	-	95,105,120,121	0
2	GD3	A	601	1/1	0.97	0.07	-	120,120,120,120	0
2	GD3	B	601	1/1	1.00	0.10	-	107,107,107,107	0
6	NAG	B	606	14/15	0.86	0.29	-	88,112,125,126	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
6	NAG	B	607	14/15	0.89	0.31	-	109,121,131,133	0
6	NAG	A	606	14/15	0.84	0.42	-	93,124,141,144	0

6.5 Other polymers

There are no such residues in this entry.