



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:05 PM UTC

PDB ID : 5FBK / pdb_00005fbk
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

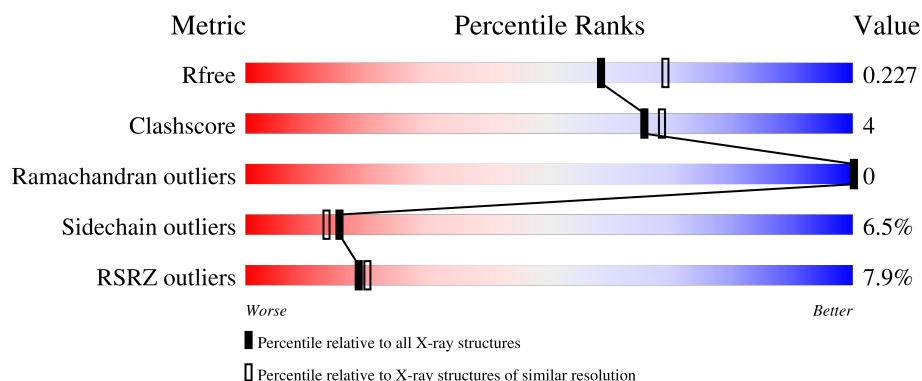
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	9% 78% 6% 14%
1	B	568	4% 72% 7% 18%

2 Entry composition

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
1	A	487	Total	C	N	O	S	0	0	0
			3778	2424	631	710	13			
1	B	467	Total	C	N	O	S	0	0	0
			3639	2335	615	677	12			

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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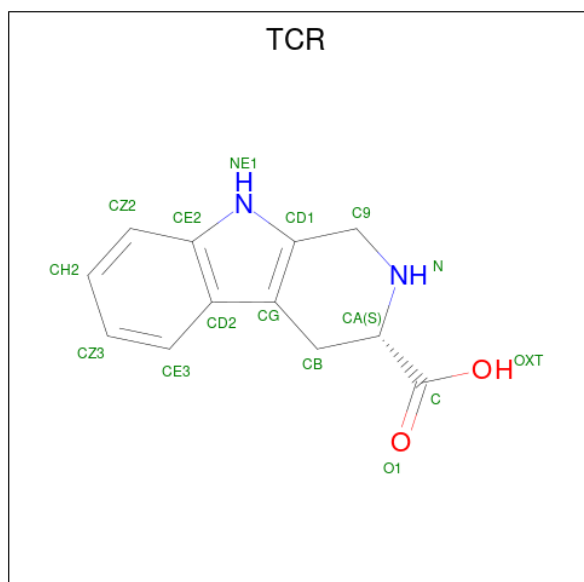
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P41180
A	0	HIS	-	expression tag	UNP P41180
A	1	HIS	-	expression tag	UNP P41180
A	2	HIS	-	expression tag	UNP P41180
A	3	HIS	-	expression tag	UNP P41180
A	4	HIS	-	expression tag	UNP P41180
A	5	HIS	-	expression tag	UNP P41180
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 (CCD ID: TCR) (formula: $C_{12}H_{12}N_2O_2$).



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

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

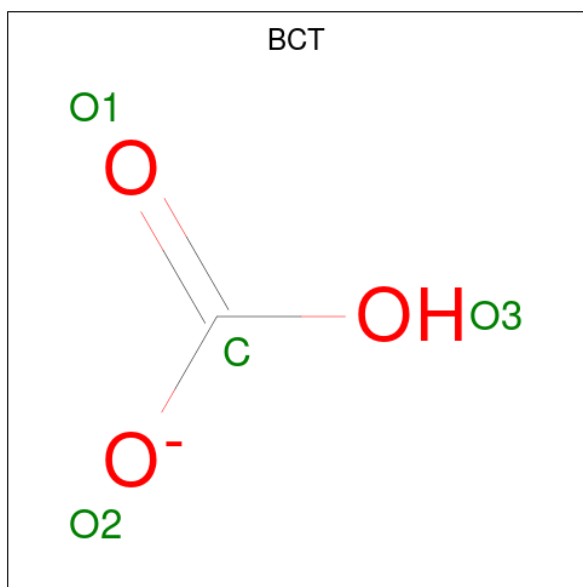


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is water.

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

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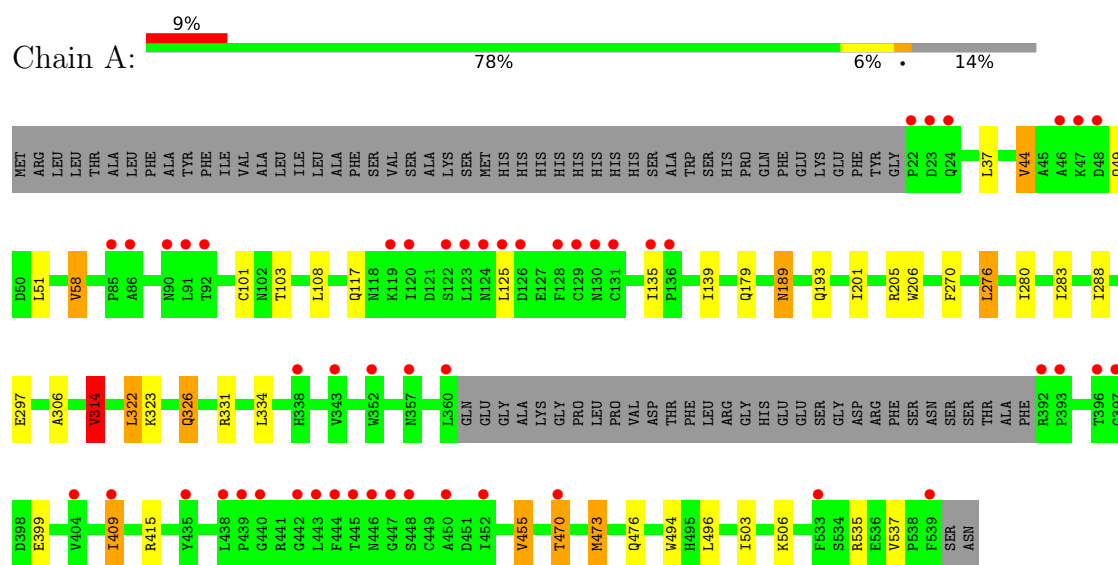
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	170	Total 170	O 170	0	0

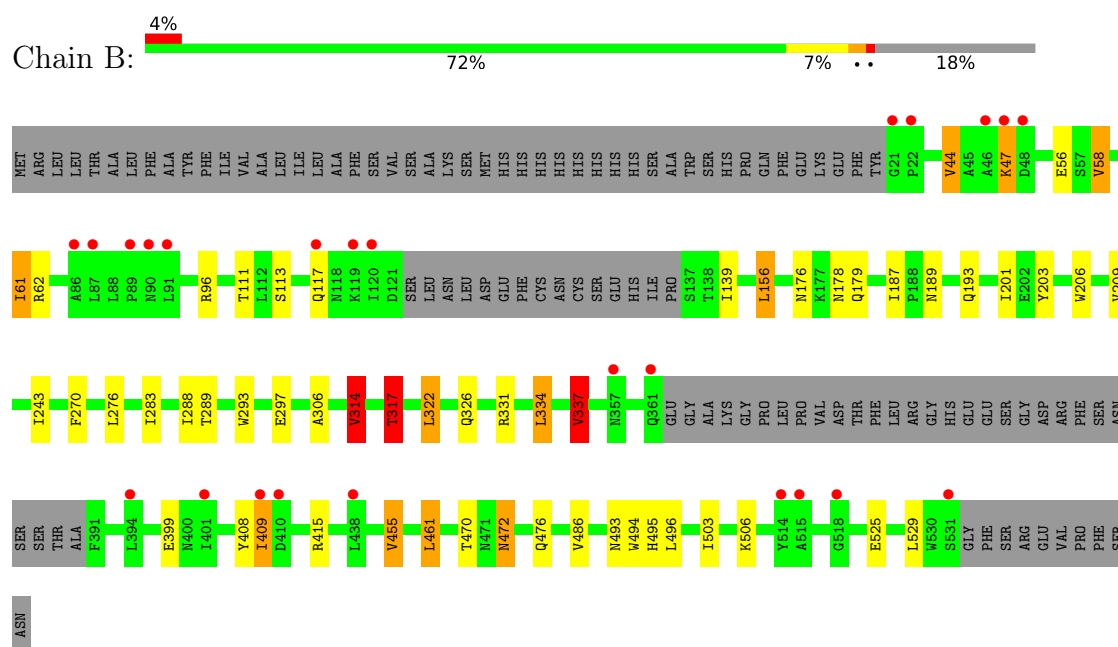
3 Residue-property plots [i](#)

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



- Molecule 1: Extracellular calcium-sensing receptor



4 Data and refinement statistics

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) 99.9 (37.77-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.190 , 0.223 (Not available) , 0.227	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 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, BCT, NAG, MG, TCR, 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	0.65	0/3854	0.82	2/5241 (0.0%)
1	B	0.71	0/3712	0.86	6/5042 (0.1%)
All	All	0.68	0/7566	0.84	8/10283 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	VAL	CB-CA-C	-7.56	99.00	111.32
1	B	189	ASN	N-CA-CB	-6.42	100.53	109.97
1	B	317	THR	N-CA-CB	6.13	119.09	109.83
1	A	314	VAL	N-CA-CB	-6.12	105.47	112.21
1	B	314	VAL	N-CA-CB	-5.75	105.89	112.21
1	B	209	VAL	N-CA-C	5.27	116.29	108.65
1	B	455	VAL	CB-CA-C	-5.27	103.25	111.26
1	A	455	VAL	CB-CA-C	-5.11	103.49	111.26

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3581	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3639	0	3475	36	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
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	7182	56	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 (56) 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:B:176:ASN:C	1:B:176:ASN:HD22	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:203:TYR:OH	1:B:525:GLU:OE2	2.21	0.51
1:B:297:GLU:HB3	7:B:746:HOH:O	2.10	0.51
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:525:GLU:H	1:B:525:GLU:CD	2.21	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:A:326:GLN:HB2	1:A:473:MET:HE1	1.96	0.46
1:B:331:ARG:NH2	1:B:409:ILE:O	2.49	0.46
1:A:189:ASN:C	1:A:189:ASN:OD1	2.58	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:306:ALA:C	1:B:503:ILE:HD12	2.42	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: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:B:243:ILE:HD12	1:B:276:LEU:HA	2.02	0.41
1:A:306:ALA:C	1:A:503:ILE:HD12	2.46	0.41

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	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

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%)	364 (93%)	26 (7%)	15	12
1	B	377/487 (77%)	353 (94%)	24 (6%)	16	14
All	All	767/974 (79%)	717 (94%)	50 (6%)	15	13

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	44	VAL
1	A	49	GLN
1	A	58	VAL
1	A	108	LEU
1	A	125	LEU
1	A	139	ILE
1	A	179	GLN

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Mol	Chain	Res	Type
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	399	GLU
1	A	409	ILE
1	A	455	VAL
1	A	470	THR
1	A	473	MET
1	A	496	LEU
1	A	506	LYS
1	A	535	ARG
1	A	537	VAL
1	B	44	VAL
1	B	47	LYS
1	B	56	GLU
1	B	58	VAL
1	B	61	ILE
1	B	117	GLN
1	B	139	ILE
1	B	156	LEU
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	326	GLN
1	B	334	LEU
1	B	337	VAL
1	B	399	GLU
1	B	409	ILE
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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	72	GLN
1	A	117	GLN
1	A	179	GLN
1	A	193	GLN
1	A	338	HIS
1	A	446	ASN
1	A	463	HIS
1	A	493	ASN
1	A	495	HIS
1	B	72	GLN
1	B	117	GLN
1	B	176	ASN
1	B	179	GLN
1	B	192	HIS
1	B	193	GLN
1	B	338	HIS
1	B	357	ASN
1	B	359	HIS
1	B	472	ASN
1	B	476	GLN
1	B	493	ASN
1	B	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	482	1	3,6,7	0.42	0	1,6,8	0.35	0
1	CSO	B	236	1	3,6,7	0.78	0	1,6,8	0.26	0
1	CSO	A	236	1	3,6,7	0.69	0	1,6,8	0.28	0
1	CSO	B	482	1	3,6,7	0.45	0	1,6,8	0.23	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
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	-
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 oligosaccharides 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	B	603	1	14,14,15	0.61	0	17,19,21	1.34	2 (11%)
3	NAG	A	603	1	14,14,15	0.53	0	17,19,21	1.35	1 (5%)
3	NAG	A	605	1	14,14,15	0.47	0	17,19,21	1.26	1 (5%)
2	TCR	A	601	-	18,18,18	2.03	3 (16%)	23,26,26	1.77	7 (30%)
3	NAG	A	604	1	14,14,15	0.55	0	17,19,21	1.57	4 (23%)
2	TCR	B	601	-	18,18,18	2.19	3 (16%)	23,26,26	1.73	6 (26%)
5	BCT	A	609	-	3,3,3	1.38	0	2,3,3	0.57	0
3	NAG	B	605	1	14,14,15	0.72	1 (7%)	17,19,21	1.24	2 (11%)
3	NAG	B	604	1	14,14,15	0.79	1 (7%)	17,19,21	1.06	0
3	NAG	A	602	1	14,14,15	0.53	0	17,19,21	2.40	5 (29%)
5	BCT	B	609	-	3,3,3	0.62	0	2,3,3	0.97	0
3	NAG	B	602	1	14,14,15	0.44	0	17,19,21	0.96	1 (5%)

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	B	603	1	-	0/6/23/26	0/1/1/1
3	NAG	A	603	1	-	2/6/23/26	0/1/1/1
3	NAG	A	605	1	-	2/6/23/26	0/1/1/1
2	TCR	A	601	-	-	0/4/13/13	0/3/3/3
3	NAG	A	604	1	-	1/6/23/26	0/1/1/1
2	TCR	B	601	-	-	2/4/13/13	0/3/3/3
3	NAG	B	605	1	-	0/6/23/26	0/1/1/1
3	NAG	B	604	1	-	0/6/23/26	0/1/1/1
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TCR	CD2-CE2	5.86	1.48	1.41
2	A	601	TCR	CD2-CE2	5.69	1.48	1.41
2	B	601	TCR	CD1-CG	4.83	1.46	1.37
2	A	601	TCR	CD1-CG	4.68	1.46	1.37
2	B	601	TCR	CE2-NE1	-2.55	1.34	1.38
2	A	601	TCR	CD2-CG	2.51	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	604	NAG	C1-C2	2.21	1.55	1.52
3	B	605	NAG	C1-C2	2.08	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAG	C1-O5-C5	7.63	122.41	112.19
2	A	601	TCR	CZ2-CE2-CD2	-4.14	118.18	122.19
3	A	603	NAG	C1-O5-C5	3.94	117.46	112.19
2	B	601	TCR	C9-CD1-NE1	3.86	128.13	124.20
3	A	605	NAG	C1-O5-C5	3.75	117.22	112.19
2	B	601	TCR	CZ2-CE2-CD2	-3.45	118.84	122.19
3	A	604	NAG	C3-C4-C5	3.33	116.27	110.23
3	A	604	NAG	O5-C1-C2	-3.31	106.17	111.29
3	A	602	NAG	O5-C5-C4	3.29	118.84	110.83
2	A	601	TCR	C9-CD1-NE1	3.21	127.47	124.20
3	A	602	NAG	C3-C4-C5	2.96	115.60	110.23
2	A	601	TCR	CD2-CG-CD1	-2.95	104.01	106.88
2	B	601	TCR	CE3-CD2-CE2	2.75	121.69	118.84
3	B	603	NAG	C1-O5-C5	2.72	115.84	112.19
2	B	601	TCR	CD2-CG-CD1	-2.62	104.33	106.88
2	B	601	TCR	CB-CA-C	-2.54	106.17	112.06
2	A	601	TCR	CE3-CD2-CE2	2.51	121.44	118.84
3	B	602	NAG	O5-C1-C2	-2.49	107.44	111.29
3	B	605	NAG	O5-C5-C4	-2.38	105.04	110.83
3	B	605	NAG	C3-C4-C5	-2.30	106.07	110.23
3	B	603	NAG	O3-C3-C4	-2.27	105.02	110.38
2	A	601	TCR	CE2-NE1-CD1	2.26	111.50	108.98
2	A	601	TCR	C-CA-N	-2.12	105.80	108.97
2	B	601	TCR	CE2-NE1-CD1	2.04	111.26	108.98
2	A	601	TCR	OXT-C-CA	2.03	120.36	113.51
3	A	602	NAG	O5-C1-C2	-2.02	108.17	111.29
3	A	604	NAG	C4-C3-C2	2.01	113.97	111.02
3	A	604	NAG	C1-O5-C5	2.01	114.88	112.19
3	A	602	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (7) 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

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Mol	Chain	Res	Type	Atoms
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
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

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	485/568 (85%)	0.58	51 (10%)	11 12	25, 45, 86, 109	0
1	B	465/568 (81%)	0.26	24 (5%)	33 35	23, 40, 68, 89	0
All	All	950/1136 (83%)	0.42	75 (7%)	18 20	23, 42, 77, 109	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	GLY	4.7
1	A	22	PRO	4.6
1	B	46	ALA	4.5
1	A	129	CYS	4.1
1	A	123	LEU	4.1
1	A	46	ALA	4.0
1	A	125	LEU	4.0
1	A	360	LEU	4.0
1	A	120	ILE	3.7
1	A	440	GLY	3.7
1	A	23	ASP	3.6
1	B	48	ASP	3.5
1	A	135	ILE	3.4
1	A	126	ASP	3.3
1	A	447	GLY	3.3
1	B	86	ALA	3.3
1	A	136	PRO	3.2
1	A	90	ASN	3.2
1	A	86	ALA	3.2
1	B	514	TYR	3.2
1	A	124	ASN	3.2
1	A	128	PHE	3.1
1	A	404	VAL	3.1
1	A	85	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	120	ILE	3.0
1	B	438	LEU	3.0
1	A	445	THR	3.0
1	B	22	PRO	2.9
1	A	396	THR	2.9
1	B	394	LEU	2.8
1	A	122	SER	2.8
1	B	531	SER	2.8
1	B	119	LYS	2.8
1	B	515	ALA	2.8
1	A	533	PHE	2.7
1	B	47	LYS	2.6
1	A	91	LEU	2.6
1	A	452	ILE	2.6
1	A	48	ASP	2.6
1	A	435	TYR	2.6
1	B	401	ILE	2.5
1	A	92	THR	2.5
1	A	47	LYS	2.5
1	A	357	ASN	2.5
1	B	357	ASN	2.5
1	A	450	ALA	2.5
1	B	361	GLN	2.5
1	A	409	ILE	2.5
1	B	117	GLN	2.4
1	A	448	SER	2.4
1	A	119	LYS	2.4
1	A	439	PRO	2.4
1	A	24	GLN	2.4
1	A	444	PHE	2.3
1	A	393	PRO	2.3
1	B	90	ASN	2.3
1	A	470	THR	2.3
1	A	446	ASN	2.3
1	A	343	VAL	2.2
1	A	392	ARG	2.2
1	A	443	LEU	2.2
1	A	352	TRP	2.2
1	A	130	ASN	2.2
1	B	410	ASP	2.2
1	A	131	CYS	2.2
1	B	409	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	87	LEU	2.1
1	A	442	GLY	2.1
1	B	518	GLY	2.1
1	B	91	LEU	2.1
1	A	338	HIS	2.1
1	A	438	LEU	2.0
1	B	89	PRO	2.0
1	A	539	PHE	2.0
1	A	397	GLY	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	B	482	7/8	0.89	0.12	35,37,54,56	0
1	CSO	A	236	7/8	0.93	0.09	37,37,44,49	0
1	CSO	A	482	7/8	0.95	0.07	32,35,45,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	0.52	0.16	91,101,104,106	0
3	NAG	A	604	14/15	0.63	0.15	75,88,92,92	0
3	NAG	B	605	14/15	0.70	0.14	74,86,100,107	0
3	NAG	A	602	14/15	0.73	0.13	62,66,73,76	0
3	NAG	A	605	14/15	0.76	0.13	62,75,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	603	14/15	0.78	0.12	79,82,87,87	0
3	NAG	B	602	14/15	0.87	0.11	47,60,65,67	0
3	NAG	B	603	14/15	0.90	0.10	46,48,54,54	0
6	MG	A	610	1/1	0.91	0.07	56,56,56,56	0
4	CL	A	608	1/1	0.93	0.12	57,57,57,57	0
4	CL	B	608	1/1	0.94	0.16	58,58,58,58	0
5	BCT	B	609	4/4	0.95	0.09	28,33,35,38	0
6	MG	B	611	1/1	0.95	0.09	57,57,57,57	0
5	BCT	A	609	4/4	0.96	0.06	34,36,36,40	0
2	TCR	B	601	16/16	0.96	0.07	23,35,43,46	0
2	TCR	A	601	16/16	0.97	0.06	25,33,39,40	0
4	CL	A	606	1/1	0.98	0.06	42,42,42,42	0
4	CL	B	606	1/1	0.98	0.08	43,43,43,43	0
4	CL	B	607	1/1	0.98	0.28	49,49,49,49	0
6	MG	B	610	1/1	0.98	0.06	45,45,45,45	0
4	CL	A	607	1/1	0.98	0.22	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.