



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:12 pm GMT

PDB ID : 5K5S
Title : Crystal structure of the active form of human calcium-sensing receptor extra-cellular domain
Authors : Geng, Y.; Mosyak, L.; Kurinov, I.; Zuo, H.; Sturchler, E.; Cheng, T.C.; Subramanyam, P.; Brown, A.P.; Brennan, S.C.; Mun, H.-C.; Bush, M.; Chen, Y.; Nguyen, T.; Cao, B.; Chang, D.; Quick, M.; Conigrave, A.; Colecraft, H.M.; McDonald, P.; Fan, Q.R.
Deposited on : 2016-05-23
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

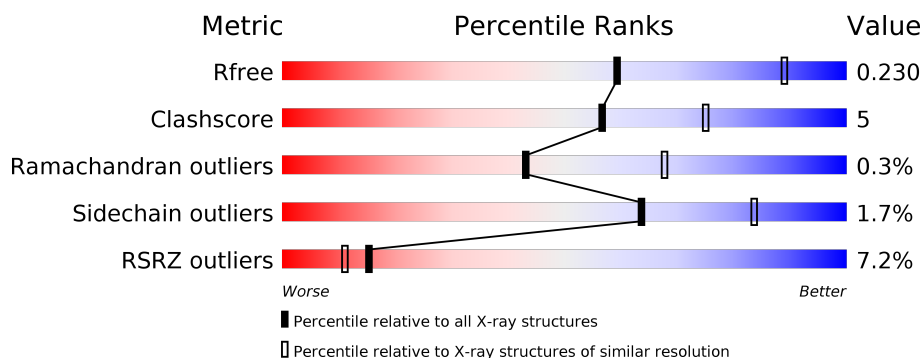
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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	615	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>14%</div> </div> </div>
1	B	615	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>13%</div> </div> </div>

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
4	CA	A	707	-	-	-	X
4	CA	A	712	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8913 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	531	Total	C	N	O	S	0	0	0
			4203	2675	707	800	21			
1	B	537	Total	C	N	O	S	0	0	0
			4251	2703	717	810	21			

There are 60 discrepancies between the modelled and reference sequences:

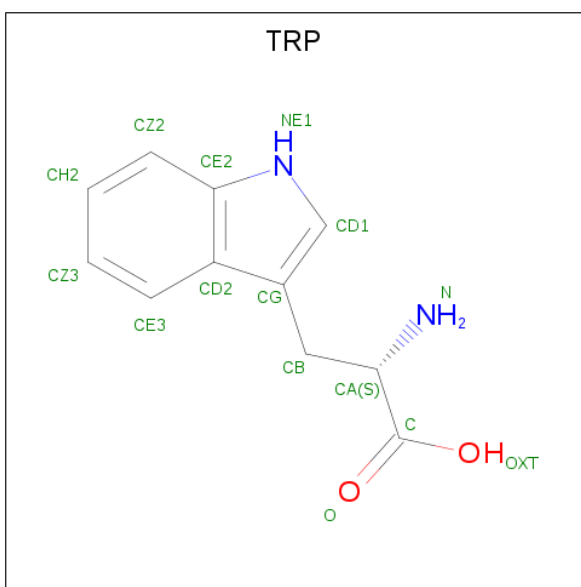
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P41180
A	2	ALA	-	expression tag	UNP P41180
A	3	PHE	-	expression tag	UNP P41180
A	4	TYR	-	expression tag	UNP P41180
A	5	SER	-	expression tag	UNP P41180
A	6	CYS	-	expression tag	UNP P41180
A	7	CYS	-	expression tag	UNP P41180
A	8	TRP	-	expression tag	UNP P41180
A	9	VAL	-	expression tag	UNP P41180
A	10	LEU	-	expression tag	UNP P41180
A	11	LEU	-	expression tag	UNP P41180
A	12	ALA	-	expression tag	UNP P41180
A	13	LEU	-	expression tag	UNP P41180
A	14	THR	-	expression tag	UNP P41180
A	15	TRP	-	expression tag	UNP P41180
A	16	HIS	-	expression tag	UNP P41180
A	17	THR	-	expression tag	UNP P41180
A	18	SER	-	expression tag	UNP P41180
A	19	ALA	-	expression tag	UNP P41180
A	386	GLN	ASN	engineered mutation	UNP P41180
A	402	ASN	SER	engineered mutation	UNP P41180
A	468	GLN	ASN	engineered mutation	UNP P41180
A	608	ASP	-	expression tag	UNP P41180
A	609	TYR	-	expression tag	UNP P41180
A	610	LYS	-	expression tag	UNP P41180

Continued on next page...

Continued from previous page...

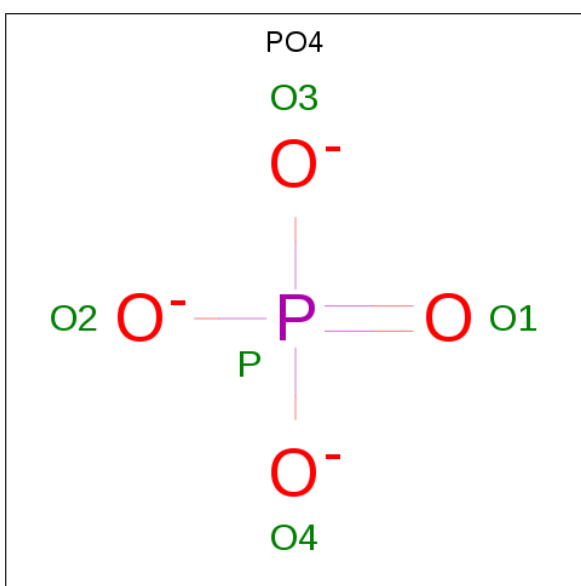
Chain	Residue	Modelled	Actual	Comment	Reference
A	611	ASP	-	expression tag	UNP P41180
A	612	ASP	-	expression tag	UNP P41180
A	613	ASP	-	expression tag	UNP P41180
A	614	ASP	-	expression tag	UNP P41180
A	615	LYS	-	expression tag	UNP P41180
B	1	MET	-	initiating methionine	UNP P41180
B	2	ALA	-	expression tag	UNP P41180
B	3	PHE	-	expression tag	UNP P41180
B	4	TYR	-	expression tag	UNP P41180
B	5	SER	-	expression tag	UNP P41180
B	6	CYS	-	expression tag	UNP P41180
B	7	CYS	-	expression tag	UNP P41180
B	8	TRP	-	expression tag	UNP P41180
B	9	VAL	-	expression tag	UNP P41180
B	10	LEU	-	expression tag	UNP P41180
B	11	LEU	-	expression tag	UNP P41180
B	12	ALA	-	expression tag	UNP P41180
B	13	LEU	-	expression tag	UNP P41180
B	14	THR	-	expression tag	UNP P41180
B	15	TRP	-	expression tag	UNP P41180
B	16	HIS	-	expression tag	UNP P41180
B	17	THR	-	expression tag	UNP P41180
B	18	SER	-	expression tag	UNP P41180
B	19	ALA	-	expression tag	UNP P41180
B	386	GLN	ASN	engineered mutation	UNP P41180
B	402	ASN	SER	engineered mutation	UNP P41180
B	468	GLN	ASN	engineered mutation	UNP P41180
B	608	ASP	-	expression tag	UNP P41180
B	609	TYR	-	expression tag	UNP P41180
B	610	LYS	-	expression tag	UNP P41180
B	611	ASP	-	expression tag	UNP P41180
B	612	ASP	-	expression tag	UNP P41180
B	613	ASP	-	expression tag	UNP P41180
B	614	ASP	-	expression tag	UNP P41180
B	615	LYS	-	expression tag	UNP P41180

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

Continued on next page...

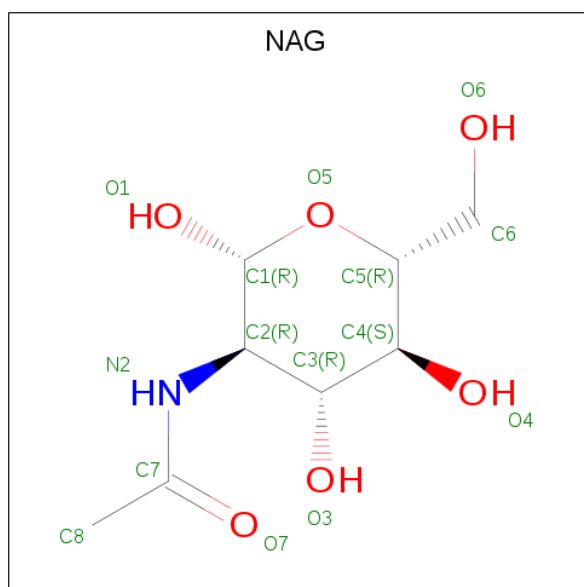
Continued from previous page...

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Ca	0	0
			3	3		
4	A	5	Total	Ca	0	0
			5	5		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

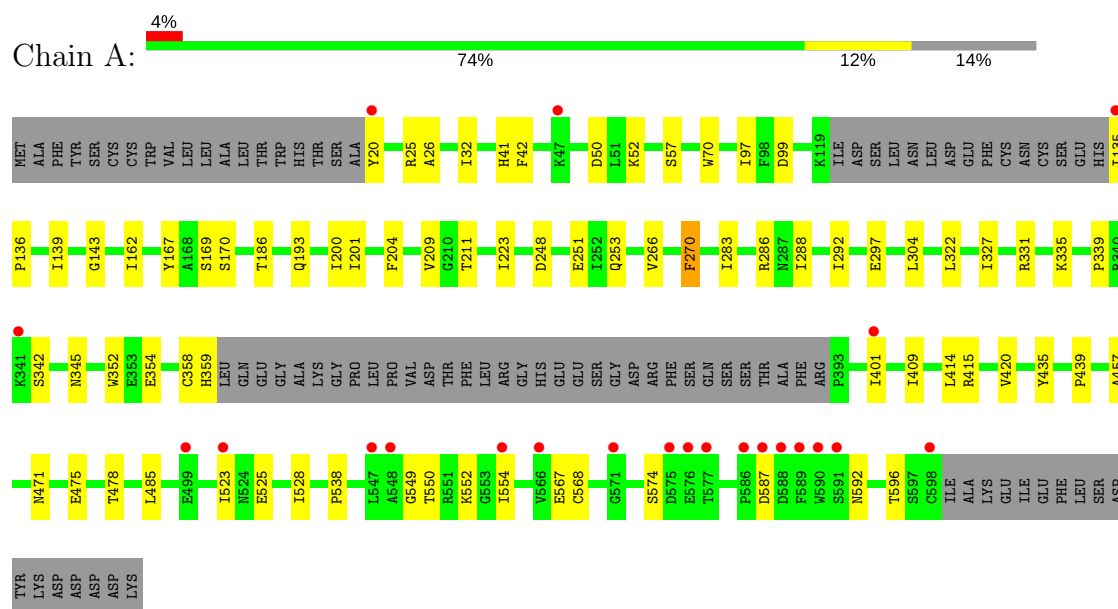
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	189	Total 189	O 189	0	0
6	B	142	Total 142	O 142	0	0

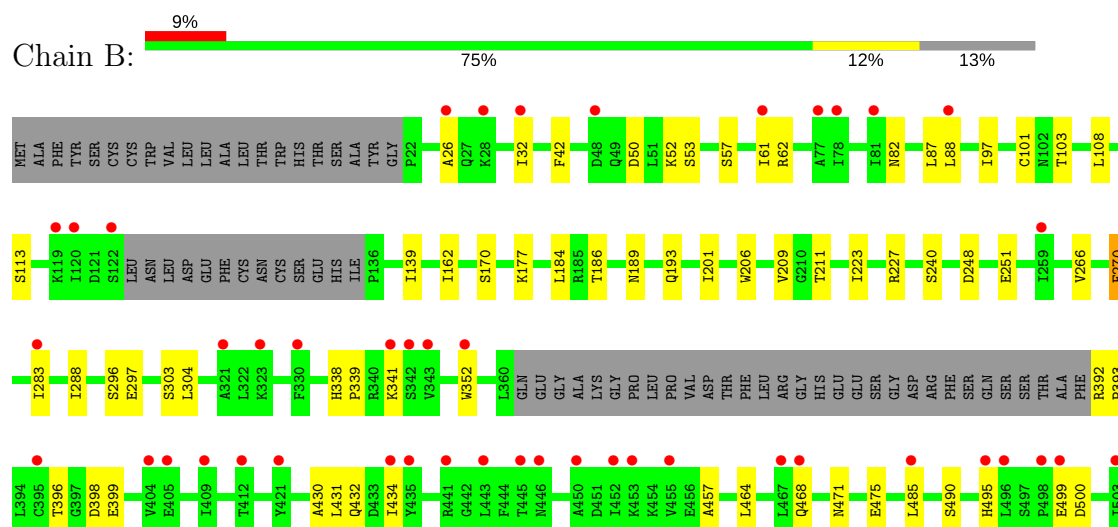
3 Residue-property plots

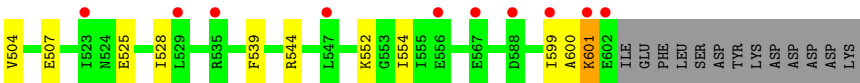
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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	107.66Å 127.45Å 146.77Å 90.00° 108.72° 90.00°	Depositor
Resolution (Å)	38.07 – 2.60 139.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.7 (38.07-2.60) 84.8 (139.01-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.211 , 0.222 0.219 , 0.230	Depositor DCC
R_{free} test set	2476 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 76.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8913	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 3.35% 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: PO4, CA, NAG

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	0.44	0/4305	0.69	0/5837
1	B	0.45	0/4352	0.71	0/5898
All	All	0.45	0/8657	0.70	0/11735

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	GLU	Sidechain
1	B	189	ASN	Sidechain

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	4203	0	4037	47	0
1	B	4251	0	4097	42	0
2	A	15	0	9	4	0
2	B	15	0	9	3	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
5	A	56	0	52	0	0
5	B	14	0	13	0	0
6	A	189	0	0	1	0
6	B	142	0	0	2	0
All	All	8913	0	8217	91	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 5.

All (91) 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:253:GLN:HE22	1:A:286:ARG:HH11	0.97	0.96
1:A:193:GLN:HE22	1:A:297:GLU:H	1.20	0.88
1:B:193:GLN:HE22	1:B:297:GLU:H	1.22	0.86
1:A:253:GLN:HE22	1:A:286:ARG:NH1	1.73	0.85
1:A:253:GLN:NE2	1:A:286:ARG:HH11	1.75	0.85
1:A:335:LYS:HA	1:A:401:ILE:HD11	1.60	0.83
1:A:32:ILE:HG23	1:A:139:ILE:HG12	1.66	0.77
2:A:701:TRP:CD1	2:A:701:TRP:N	2.54	0.75
1:B:32:ILE:HG23	1:B:139:ILE:HG12	1.69	0.75
1:A:331:ARG:HH22	1:A:409:ILE:HG23	1.54	0.72
1:A:554:ILE:HD12	1:B:552:LYS:HB3	1.71	0.71
2:A:701:TRP:N	2:A:701:TRP:HD1	1.89	0.69
1:A:20:TYR:HB3	1:A:25:ARG:HH22	1.59	0.68
1:B:338:HIS:HB3	1:B:341:LYS:HB2	1.78	0.66
1:B:227:ARG:NH1	1:B:240:SER:HB3	2.12	0.65
1:A:253:GLN:NE2	1:A:286:ARG:NH1	2.41	0.62
2:B:701:TRP:CD1	2:B:701:TRP:N	2.67	0.62
1:B:209:VAL:HG12	1:B:266:VAL:HB	1.81	0.61
1:B:227:ARG:HH12	1:B:240:SER:HB3	1.64	0.60
1:B:61:ILE:HG22	1:B:62:ARG:HG3	1.83	0.60
1:A:331:ARG:NH2	1:A:409:ILE:HG23	2.15	0.60
1:A:209:VAL:HG12	1:A:266:VAL:HB	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:HIS:HD2	1:A:99:ASP:OD2	1.85	0.59
1:B:186:THR:HA	1:B:485:LEU:HD21	1.83	0.59
1:B:193:GLN:HE22	1:B:297:GLU:N	1.97	0.59
1:B:87:LEU:HA	1:B:432:GLN:OE1	2.02	0.59
1:A:266:VAL:HG22	1:A:292:ILE:HD11	1.84	0.59
1:A:170:SER:HG	2:A:701:TRP:N	2.01	0.58
1:A:50:ASP:HB2	1:A:52:LYS:HG3	1.85	0.58
1:B:82:ASN:HA	6:B:801:HOH:O	2.04	0.57
1:A:169:SER:HA	2:A:701:TRP:OXT	2.05	0.56
1:A:552:LYS:HB3	1:B:554:ILE:HD12	1.88	0.55
1:A:549:GLY:H	1:A:574:SER:HB3	1.71	0.54
1:B:339:PRO:HD3	1:B:352:TRP:CE2	2.43	0.53
1:A:186:THR:HA	1:A:485:LEU:HD12	1.89	0.53
1:B:170:SER:HG	2:B:701:TRP:N	2.07	0.53
2:B:701:TRP:HD1	2:B:701:TRP:N	2.06	0.53
1:A:568:CYS:SG	1:A:574:SER:HB2	2.49	0.52
1:A:211:THR:HB	1:A:223:ILE:HD12	1.92	0.52
1:A:193:GLN:HE22	1:A:297:GLU:N	1.99	0.52
1:B:211:THR:HB	1:B:223:ILE:HD12	1.90	0.52
1:A:26:ALA:HB3	1:A:97:ILE:HB	1.93	0.51
1:B:50:ASP:HB2	1:B:52:LYS:HG3	1.94	0.50
1:A:201:ILE:HD13	1:A:209:VAL:HG11	1.93	0.50
1:B:184:LEU:HD11	1:B:464:LEU:HB3	1.93	0.49
1:A:200:ILE:HG12	1:A:523:ILE:HD11	1.93	0.49
1:B:600:ALA:O	1:B:601:LYS:HB2	2.13	0.49
1:B:26:ALA:HB3	1:B:97:ILE:HB	1.95	0.49
1:B:201:ILE:HD13	1:B:209:VAL:HG11	1.94	0.48
1:B:471:ASN:HB3	1:B:475:GLU:H	1.78	0.48
1:B:223:ILE:HG12	1:B:270:PHE:HB2	1.95	0.48
1:A:478:THR:O	1:A:485:LEU:HD23	2.14	0.48
1:B:352:TRP:CZ3	1:B:399:GLU:HB2	2.48	0.48
1:B:468:GLN:HB3	6:B:819:HOH:O	2.14	0.48
1:A:292:ILE:HG21	1:A:538:PRO:HG2	1.96	0.47
1:A:550:THR:HG22	1:A:567:GLU:HA	1.95	0.47
1:B:101:CYS:O	1:B:103:THR:HG23	2.15	0.47
1:A:248:ASP:HB2	1:A:251:GLU:H	1.80	0.47
1:B:177:LYS:HD3	1:B:177:LYS:HA	1.71	0.46
1:A:223:ILE:HG12	1:A:270:PHE:HB2	1.97	0.45
1:A:525:GLU:HA	1:A:528:ILE:HD12	1.98	0.45
1:A:283:ILE:HG23	1:A:288:ILE:HB	1.97	0.45
1:B:248:ASP:HB2	1:B:251:GLU:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:HD13	1:B:431:LEU:HD22	1.98	0.45
1:A:471:ASN:HB3	1:A:475:GLU:H	1.82	0.45
1:B:539:PHE:CZ	1:B:544:ARG:HD2	2.51	0.45
1:A:292:ILE:HA	6:A:802:HOH:O	2.17	0.45
1:A:204:PHE:HE1	1:A:525:GLU:HG2	1.83	0.44
1:B:495:HIS:HB2	1:B:504:VAL:HG13	1.99	0.44
1:B:396:THR:C	1:B:398:ASP:H	2.22	0.44
1:B:352:TRP:HZ3	1:B:399:GLU:HB2	1.82	0.44
1:A:592:ASN:HD21	1:A:596:THR:HB	1.83	0.44
1:A:135:ILE:N	1:A:136:PRO:CD	2.81	0.43
1:B:42:PHE:CZ	1:B:304:LEU:HD11	2.53	0.43
1:B:283:ILE:HG23	1:B:288:ILE:HB	2.00	0.43
1:A:342:SER:HB3	1:A:345:ASN:HB3	1.99	0.43
1:A:162:ILE:HA	1:A:457:ALA:HB1	2.00	0.43
1:B:162:ILE:HA	1:B:457:ALA:HB1	2.00	0.43
1:B:392:ARG:N	1:B:393:PRO:HD2	2.33	0.42
1:A:322:LEU:O	1:A:415:ARG:HD3	2.19	0.42
1:B:525:GLU:HA	1:B:528:ILE:HD12	2.01	0.42
1:B:499:GLU:HG3	1:B:500:ASP:H	1.84	0.42
1:A:339:PRO:HD3	1:A:352:TRP:CD2	2.55	0.42
1:A:42:PHE:CZ	1:A:304:LEU:HD11	2.56	0.41
1:A:253:GLN:OE1	1:A:286:ARG:NH1	2.49	0.41
1:A:143:GLY:HA2	1:A:167:TYR:CE2	2.55	0.41
1:B:490:SER:OG	1:B:507:GLU:HG3	2.21	0.41
1:A:327:ILE:HD12	1:A:414:LEU:HD13	2.02	0.41
1:A:70:TRP:HB3	1:A:420:VAL:HG21	2.04	0.40
1:B:430:ALA:O	1:B:434:ILE:HG12	2.21	0.40
1:B:201:ILE:HG23	1:B:206:TRP:HB2	2.04	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	525/615 (85%)	500 (95%)	23 (4%)	2 (0%)	36	60
1	B	531/615 (86%)	502 (94%)	28 (5%)	1 (0%)	49	74
All	All	1056/1230 (86%)	1002 (95%)	51 (5%)	3 (0%)	43	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	PRO
1	A	587	ASP
1	B	601	LYS

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	457/531 (86%)	452 (99%)	5 (1%)	76	90
1	B	463/531 (87%)	454 (98%)	9 (2%)	60	82
All	All	920/1062 (87%)	906 (98%)	14 (2%)	63	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	270	PHE
1	A	358	CYS
1	A	359	HIS
1	A	435	TYR
1	B	53	SER
1	B	57	SER
1	B	88	LEU
1	B	108	LEU
1	B	113	SER
1	B	270	PHE
1	B	296	SER
1	B	303	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	599	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	72	GLN
1	A	193	GLN
1	B	193	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 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	$\# Z > 2$
2	TRP	A	701	-	11,16,16	0.61	0	11,22,22	0.84	0
3	PO4	A	702	-	4,4,4	1.77	0	6,6,6	0.76	0
3	PO4	A	703	-	4,4,4	2.08	1 (25%)	6,6,6	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	708	1	14,14,15	0.30	0	17,19,21	0.66	0
5	NAG	A	709	1	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
5	NAG	A	710	1	14,14,15	0.34	0	17,19,21	1.48	4 (23%)
5	NAG	A	711	1	14,14,15	0.25	0	17,19,21	1.00	1 (5%)
2	TRP	B	701	-	11,16,16	0.63	0	11,22,22	0.82	0
3	PO4	B	702	-	4,4,4	1.89	1 (25%)	6,6,6	0.93	0
3	PO4	B	703	-	4,4,4	2.12	1 (25%)	6,6,6	0.31	0
5	NAG	B	707	1	14,14,15	0.42	0	17,19,21	2.44	3 (17%)

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
2	TRP	A	701	-	-	0/3/8/8	0/2/2/2
3	PO4	A	702	-	-	0/0/0/0	0/0/0/0
3	PO4	A	703	-	-	0/0/0/0	0/0/0/0
5	NAG	A	708	1	-	0/6/23/26	0/1/1/1
5	NAG	A	709	1	-	0/6/23/26	0/1/1/1
5	NAG	A	710	1	-	0/6/23/26	0/1/1/1
5	NAG	A	711	1	-	0/6/23/26	0/1/1/1
2	TRP	B	701	-	-	0/3/8/8	0/2/2/2
3	PO4	B	702	-	-	0/0/0/0	0/0/0/0
3	PO4	B	703	-	-	0/0/0/0	0/0/0/0
5	NAG	B	707	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	PO4	P-O3	2.02	1.61	1.54
3	B	703	PO4	P-O1	2.87	1.57	1.50
3	A	703	PO4	P-O1	2.97	1.57	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	710	NAG	C1-C2-N2	-3.37	104.73	110.49
5	A	711	NAG	C1-C2-N2	-3.35	104.76	110.49
5	A	709	NAG	O5-C1-C2	-3.21	107.09	111.52
5	A	710	NAG	O5-C1-C2	-2.33	108.31	111.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	710	NAG	C1-O5-C5	2.14	115.13	112.19
5	B	707	NAG	C2-N2-C7	3.01	127.33	122.94
5	A	710	NAG	C2-N2-C7	3.33	127.80	122.94
5	B	707	NAG	C1-C2-N2	5.51	119.91	110.49
5	B	707	NAG	C1-O5-C5	7.23	122.13	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	TRP	4	0
2	B	701	TRP	3	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	531/615 (86%)	0.65	22 (4%) 37 29	20, 53, 133, 211	0
1	B	537/615 (87%)	0.85	55 (10%) 7 4	31, 69, 119, 157	0
All	All	1068/1230 (86%)	0.75	77 (7%) 15 11	20, 61, 126, 211	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	589	PHE	6.2
1	B	404	VAL	5.9
1	B	602	GLU	5.9
1	B	445	THR	5.7
1	A	575	ASP	5.4
1	A	20	TYR	5.2
1	B	48	ASP	4.8
1	B	446	ASN	4.4
1	B	453	LYS	4.3
1	B	468	GLN	4.2
1	A	499	GLU	4.2
1	B	499	GLU	4.2
1	A	590	TRP	4.2
1	B	441	ARG	4.1
1	B	341	LYS	3.9
1	B	498	PRO	3.9
1	A	591	SER	3.8
1	A	588	ASP	3.8
1	A	47	LYS	3.7
1	B	330	PHE	3.7
1	B	435	TYR	3.6
1	B	119	LYS	3.6
1	B	122	SER	3.4
1	A	566	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	341	LYS	3.4
1	A	587	ASP	3.3
1	A	576	GLU	3.3
1	B	77	ALA	3.3
1	B	443	LEU	3.1
1	B	452	ILE	3.1
1	B	496	LEU	3.1
1	B	405	GLU	3.1
1	A	598	CYS	3.0
1	A	547	LEU	3.0
1	B	342	SER	3.0
1	B	535	ARG	2.9
1	B	529	LEU	2.9
1	B	352	TRP	2.8
1	A	523	ILE	2.8
1	B	81	ILE	2.8
1	B	556	GLU	2.7
1	B	434	ILE	2.7
1	A	577	THR	2.7
1	B	421	TYR	2.7
1	B	78	ILE	2.6
1	B	467	LEU	2.6
1	B	88	LEU	2.6
1	A	401	ILE	2.6
1	A	548	ALA	2.6
1	A	586	PRO	2.5
1	A	554	ILE	2.5
1	B	323	LYS	2.5
1	B	61	ILE	2.5
1	B	343	VAL	2.4
1	B	588	ASP	2.3
1	B	495	HIS	2.3
1	B	485	LEU	2.3
1	B	547	LEU	2.3
1	B	455	VAL	2.3
1	B	26	ALA	2.2
1	B	395	CYS	2.2
1	B	28	LYS	2.2
1	B	601	LYS	2.2
1	A	135	ILE	2.1
1	B	283	ILE	2.1
1	B	409	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	32	ILE	2.1
1	B	321	ALA	2.1
1	B	599	ILE	2.1
1	B	450	ALA	2.1
1	B	259	ILE	2.0
1	B	503	ILE	2.0
1	B	567	GLU	2.0
1	A	571	GLY	2.0
1	B	120	ILE	2.0
1	B	523	ILE	2.0
1	B	412	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	CA	A	707	1/1	0.06	0.47	139,139,139,139	0
4	CA	A	712	1/1	0.37	0.46	140,140,140,140	0
5	NAG	A	708	14/15	0.75	0.23	88,91,94,95	0
4	CA	B	704	1/1	0.79	0.06	102,102,102,102	0
5	NAG	A	709	14/15	0.80	0.20	70,73,81,84	0
5	NAG	A	710	14/15	0.81	0.23	84,88,94,95	0
5	NAG	A	711	14/15	0.82	0.21	68,71,74,78	0
5	NAG	B	707	14/15	0.86	0.18	71,72,74,74	0
2	TRP	B	701	15/15	0.89	0.23	45,48,52,59	0
3	PO4	A	703	5/5	0.92	0.16	76,77,78,79	0
4	CA	A	706	1/1	0.93	0.13	83,83,83,83	0
3	PO4	B	703	5/5	0.93	0.16	72,72,74,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CA	B	705	1/1	0.95	0.12	81,81,81,81	0
3	PO4	B	702	5/5	0.95	0.21	59,60,60,65	0
2	TRP	A	701	15/15	0.96	0.21	18,28,30,57	0
4	CA	B	706	1/1	0.97	0.34	111,111,111,111	0
4	CA	A	705	1/1	0.97	0.15	56,56,56,56	0
4	CA	A	704	1/1	0.97	0.12	53,53,53,53	0
3	PO4	A	702	5/5	0.99	0.22	26,30,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.