



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:55 AM GMT

PDB ID : 2J9L
Title : CYTOPLASMIC DOMAIN OF THE HUMAN CHLORIDE TRANSPORTER
CLC-5 IN COMPLEX WITH ATP
Authors : Meyer, S.; Savaresi, S.; Forster, I.C.; Dutzler, R.
Deposited on : 2006-11-13
Resolution : 2.30 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

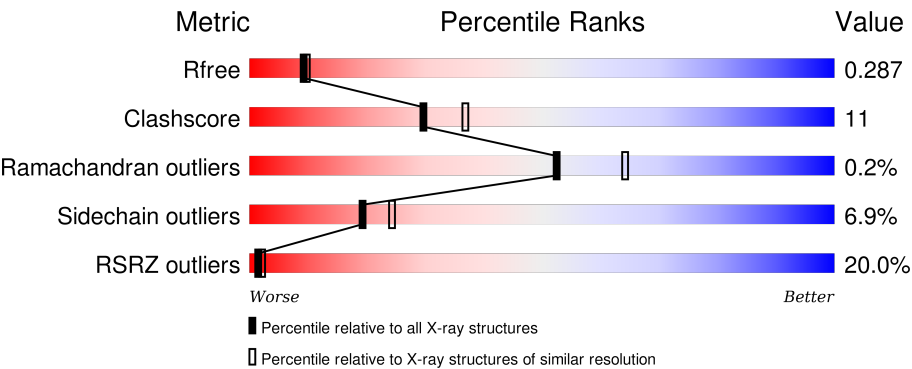
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	185	<div><div>16%</div><div><div></div><div>74%</div><div>14%</div><div>•</div><div>10%</div></div></div>
1	B	185	<div><div>11%</div><div><div></div><div>68%</div><div>22%</div><div>•</div><div>8%</div></div></div>
1	C	185	<div><div>8%</div><div><div></div><div>68%</div><div>19%</div><div>5%</div><div>•</div><div>7%</div></div></div>
1	D	185	<div><div>11%</div><div><div></div><div>69%</div><div>21%</div><div>•</div><div>8%</div></div></div>
1	E	185	<div><div>16%</div><div><div></div><div>68%</div><div>20%</div><div>•</div><div>10%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	185	<div><div></div><div>47%</div><div></div><div>75%</div><div></div><div>10%</div><div></div><div>12%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8466 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 CHLORIDE CHANNEL PROTEIN 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1326	849	226	245	6			
1	B	171	Total	C	N	O	S	0	0	0
			1362	875	231	250	6			
1	C	172	Total	C	N	O	S	0	0	0
			1371	880	233	252	6			
1	D	171	Total	C	N	O	S	0	0	0
			1353	866	231	250	6			
1	E	167	Total	C	N	O	S	0	0	0
			1326	849	226	245	6			
1	F	162	Total	C	N	O	S	0	0	0
			1265	811	217	231	6			

There are 54 discrepancies between the modelled and reference sequences:

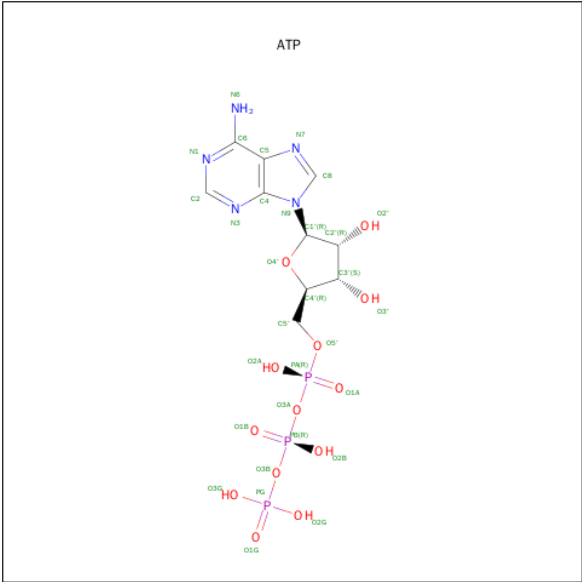
Chain	Residue	Modelled	Actual	Comment	Reference
A	570	MET	-	EXPRESSION TAG	UNP P51795
A	747	GLU	-	EXPRESSION TAG	UNP P51795
A	748	PHE	-	EXPRESSION TAG	UNP P51795
A	749	LEU	-	EXPRESSION TAG	UNP P51795
A	750	GLU	-	EXPRESSION TAG	UNP P51795
A	751	VAL	-	EXPRESSION TAG	UNP P51795
A	752	LEU	-	EXPRESSION TAG	UNP P51795
A	753	PHE	-	EXPRESSION TAG	UNP P51795
A	754	GLN	-	EXPRESSION TAG	UNP P51795
B	570	MET	-	EXPRESSION TAG	UNP P51795
B	747	GLU	-	EXPRESSION TAG	UNP P51795
B	748	PHE	-	EXPRESSION TAG	UNP P51795
B	749	LEU	-	EXPRESSION TAG	UNP P51795
B	750	GLU	-	EXPRESSION TAG	UNP P51795
B	751	VAL	-	EXPRESSION TAG	UNP P51795
B	752	LEU	-	EXPRESSION TAG	UNP P51795
B	753	PHE	-	EXPRESSION TAG	UNP P51795

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	754	GLN	-	EXPRESSION TAG	UNP P51795
C	570	MET	-	EXPRESSION TAG	UNP P51795
C	747	GLU	-	EXPRESSION TAG	UNP P51795
C	748	PHE	-	EXPRESSION TAG	UNP P51795
C	749	LEU	-	EXPRESSION TAG	UNP P51795
C	750	GLU	-	EXPRESSION TAG	UNP P51795
C	751	VAL	-	EXPRESSION TAG	UNP P51795
C	752	LEU	-	EXPRESSION TAG	UNP P51795
C	753	PHE	-	EXPRESSION TAG	UNP P51795
C	754	GLN	-	EXPRESSION TAG	UNP P51795
D	570	MET	-	EXPRESSION TAG	UNP P51795
D	747	GLU	-	EXPRESSION TAG	UNP P51795
D	748	PHE	-	EXPRESSION TAG	UNP P51795
D	749	LEU	-	EXPRESSION TAG	UNP P51795
D	750	GLU	-	EXPRESSION TAG	UNP P51795
D	751	VAL	-	EXPRESSION TAG	UNP P51795
D	752	LEU	-	EXPRESSION TAG	UNP P51795
D	753	PHE	-	EXPRESSION TAG	UNP P51795
D	754	GLN	-	EXPRESSION TAG	UNP P51795
E	570	MET	-	EXPRESSION TAG	UNP P51795
E	747	GLU	-	EXPRESSION TAG	UNP P51795
E	748	PHE	-	EXPRESSION TAG	UNP P51795
E	749	LEU	-	EXPRESSION TAG	UNP P51795
E	750	GLU	-	EXPRESSION TAG	UNP P51795
E	751	VAL	-	EXPRESSION TAG	UNP P51795
E	752	LEU	-	EXPRESSION TAG	UNP P51795
E	753	PHE	-	EXPRESSION TAG	UNP P51795
E	754	GLN	-	EXPRESSION TAG	UNP P51795
F	570	MET	-	EXPRESSION TAG	UNP P51795
F	747	GLU	-	EXPRESSION TAG	UNP P51795
F	748	PHE	-	EXPRESSION TAG	UNP P51795
F	749	LEU	-	EXPRESSION TAG	UNP P51795
F	750	GLU	-	EXPRESSION TAG	UNP P51795
F	751	VAL	-	EXPRESSION TAG	UNP P51795
F	752	LEU	-	EXPRESSION TAG	UNP P51795
F	753	PHE	-	EXPRESSION TAG	UNP P51795
F	754	GLN	-	EXPRESSION TAG	UNP P51795

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	Cl	0	0
			3	3		
3	E	1	Total	Cl	0	0
			1	1		
3	B	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	F	2	Total	Cl	0	0
			2	2		

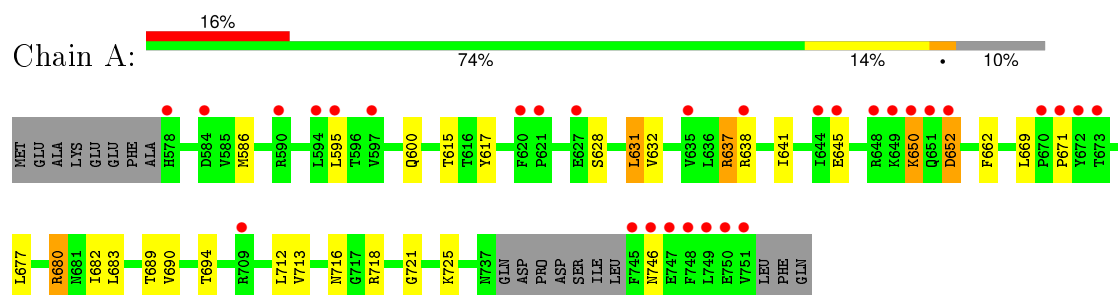
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total 43	O 43	0	0
4	B	45	Total 45	O 45	0	0
4	C	67	Total 67	O 67	0	0
4	D	58	Total 58	O 58	0	0
4	E	33	Total 33	O 33	0	0
4	F	21	Total 21	O 21	0	0

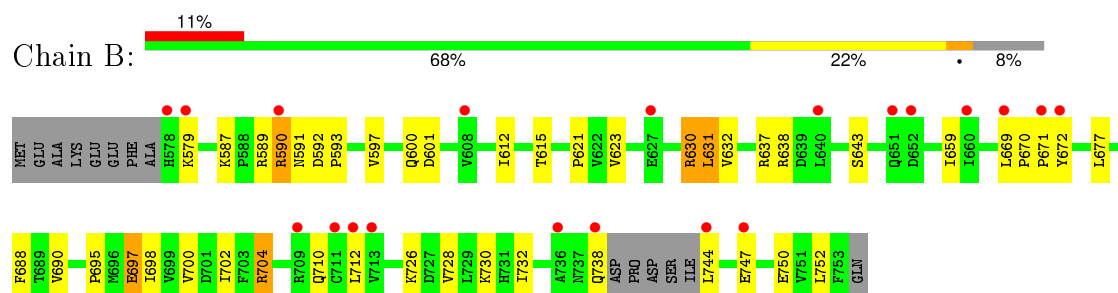
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

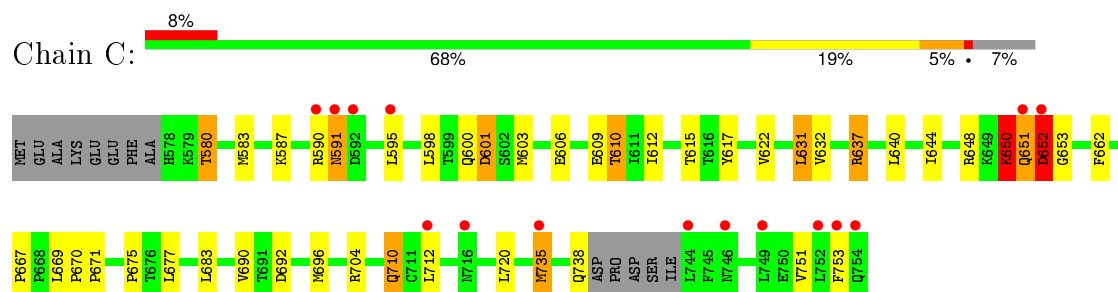
• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



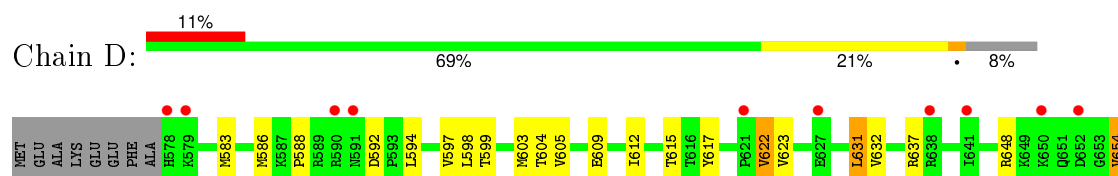
• Molecule 1: CHLORIDE CHANNEL PROTEIN 5

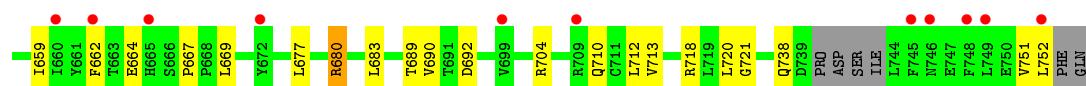


• Molecule 1: CHLORIDE CHANNEL PROTEIN 5

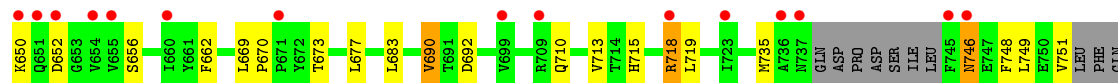
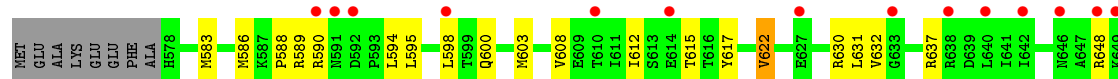


• Molecule 1: CHLORIDE CHANNEL PROTEIN 5

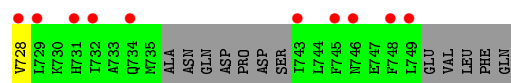
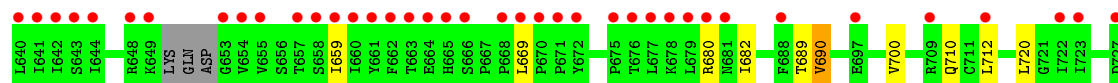
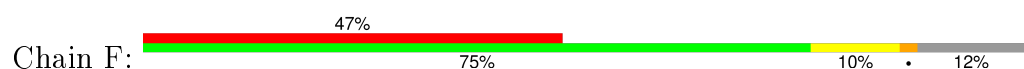




• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



• Molecule 1: CHLORIDE CHANNEL PROTEIN 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.33 Å 148.10 Å 79.88 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.30) 97.5 (19.99-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.30 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.263 , 0.295 0.260 , 0.287	Depositor DCC
R_{free} test set	3191 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 63482 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8466	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ATP, CL

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	0.31	0/1348	0.48	0/1830
1	B	0.30	0/1385	0.45	0/1880
1	C	0.32	0/1394	0.52	0/1892
1	D	0.29	0/1375	0.47	0/1867
1	E	0.26	0/1348	0.47	0/1830
1	F	0.23	0/1285	0.40	0/1745
All	All	0.29	0/8135	0.47	0/11044

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	C	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	650	LYS	Peptide
1	C	651	GLN	Peptide
1	C	652	ASP	Peptide

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	1326	0	1384	21	0
1	B	1362	0	1423	43	0
1	C	1371	0	1431	39	0
1	D	1353	0	1407	39	0
1	E	1326	0	1384	33	0
1	F	1265	0	1312	13	0
2	A	31	0	12	1	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	1	0
2	E	31	0	12	1	0
2	F	31	0	12	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	3	0	0	0	1
3	E	1	0	0	0	0
3	F	2	0	0	0	0
4	A	43	0	0	3	0
4	B	45	0	0	3	0
4	C	67	0	0	0	0
4	D	58	0	0	1	0
4	E	33	0	0	1	0
4	F	21	0	0	0	0
All	All	8466	0	8413	186	1

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 11.

All (186) 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:B:704:ARG:HG2	1:B:704:ARG:HH11	1.21	1.04
1:C:651:GLN:HB2	1:C:653:GLY:H	1.21	1.03
1:D:586:MET:CE	1:D:713:VAL:HB	1.88	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:ARG:HG2	1:B:630:ARG:HH11	1.26	1.01
1:C:651:GLN:HB2	1:C:653:GLY:N	1.80	0.95
1:D:612:ILE:O	1:D:637:ARG:NH2	2.03	0.92
1:E:617:TYR:O	1:E:637:ARG:NH1	2.03	0.91
1:B:704:ARG:CG	1:B:704:ARG:HH11	1.85	0.89
1:D:586:MET:HE3	1:D:713:VAL:CB	2.08	0.84
1:D:586:MET:HE3	1:D:713:VAL:HB	1.58	0.83
1:B:587:LYS:HD3	1:B:589:ARG:HD3	1.58	0.83
1:A:586:MET:HE3	1:A:713:VAL:HB	1.60	0.82
1:A:586:MET:CE	1:A:713:VAL:HB	2.09	0.82
1:A:586:MET:HE2	1:A:721:GLY:HA3	1.62	0.80
1:B:590:ARG:HD3	1:B:590:ARG:H	1.46	0.79
2:A:1752:ATP:O3G	4:A:2041:HOH:O	1.99	0.79
1:D:586:MET:HE2	1:D:721:GLY:HA3	1.64	0.79
1:E:622:VAL:CG1	1:E:683:LEU:HD11	2.12	0.79
1:E:622:VAL:HG11	1:E:683:LEU:HD11	1.65	0.79
1:E:622:VAL:HG11	1:E:683:LEU:CD1	2.14	0.77
1:C:644:ILE:O	1:C:648:ARG:HG3	1.84	0.77
1:D:662:PHE:O	1:D:680:ARG:HG2	1.85	0.76
1:C:609:GLU:OE1	1:C:648:ARG:NH1	2.19	0.76
1:C:606:GLU:O	1:C:610:THR:HG22	1.87	0.75
1:E:600:GLN:HE21	1:E:632:VAL:HG21	1.54	0.72
1:C:609:GLU:OE2	1:C:648:ARG:NH1	2.22	0.72
1:B:597:VAL:HG23	1:B:621:PRO:HB2	1.72	0.71
1:A:641:ILE:O	1:A:645:GLU:HB2	1.92	0.69
1:B:591:ASN:OD1	4:B:2004:HOH:O	2.09	0.69
1:B:704:ARG:HG2	1:B:704:ARG:NH1	2.00	0.68
1:A:617:TYR:O	1:A:637:ARG:NH1	2.27	0.68
1:C:650:LYS:HB3	1:C:652:ASP:OD1	1.93	0.68
1:C:609:GLU:CD	1:C:648:ARG:NH1	2.48	0.67
1:D:586:MET:HE1	1:D:713:VAL:HB	1.76	0.67
1:C:583:MET:HB3	1:C:692:ASP:HB2	1.75	0.67
1:D:605:VAL:HG21	1:D:654:VAL:HG11	1.75	0.67
1:D:609:GLU:OE1	1:D:648:ARG:NH1	2.28	0.66
1:A:586:MET:HE2	1:A:721:GLY:CA	2.24	0.66
1:D:631:LEU:HD11	1:D:712:LEU:HD12	1.76	0.65
1:C:651:GLN:CB	1:C:653:GLY:H	2.06	0.65
1:B:630:ARG:CG	1:B:630:ARG:HH11	2.06	0.65
1:A:682:ILE:O	4:A:2027:HOH:O	2.14	0.65
1:D:598:LEU:HD22	1:D:603:MET:CE	2.27	0.65
1:A:662:PHE:O	1:A:680:ARG:HG2	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:SER:OG	4:B:2024:HOH:O	2.15	0.64
1:A:586:MET:HE3	1:A:713:VAL:CB	2.27	0.64
1:D:605:VAL:HG21	1:D:654:VAL:CG1	2.27	0.63
1:D:586:MET:HE2	1:D:721:GLY:CA	2.29	0.63
1:B:697:GLU:CD	1:B:697:GLU:H	2.00	0.63
1:A:615:THR:O	1:A:637:ARG:NH2	2.32	0.62
1:D:598:LEU:HD22	1:D:603:MET:HE2	1.80	0.62
1:E:746:ASN:HB3	1:E:749:LEU:HD12	1.82	0.61
1:A:652:ASP:OD1	1:A:652:ASP:N	2.33	0.61
1:C:631:LEU:HD11	1:C:712:LEU:HD12	1.83	0.61
1:A:631:LEU:HD11	1:A:712:LEU:HD12	1.81	0.61
1:C:651:GLN:HB2	1:C:652:ASP:C	2.22	0.60
1:F:622:VAL:HG23	1:F:632:VAL:HB	1.83	0.60
1:C:704:ARG:NH2	1:C:751:VAL:O	2.34	0.60
1:F:598:LEU:HB2	1:F:622:VAL:HG12	1.83	0.60
1:B:630:ARG:HG2	1:B:630:ARG:NH1	2.04	0.59
1:A:716:ASN:O	1:B:630:ARG:HG2	2.03	0.59
1:C:612:ILE:HD11	1:C:640:LEU:HB3	1.83	0.59
1:D:586:MET:HE3	1:D:713:VAL:CG1	2.34	0.58
1:E:748:PHE:O	1:E:751:VAL:HG22	2.03	0.57
1:C:651:GLN:CB	1:C:653:GLY:N	2.63	0.57
1:E:735:MET:HB3	1:E:748:PHE:HB2	1.87	0.57
1:F:599:THR:OG1	1:F:603:MET:HG2	2.05	0.57
1:B:697:GLU:CD	1:B:697:GLU:N	2.57	0.56
1:C:591:ASN:HD22	1:C:591:ASN:C	2.08	0.56
1:E:600:GLN:NE2	1:E:632:VAL:HG21	2.21	0.56
1:B:752:LEU:HD21	1:D:752:LEU:HD23	1.87	0.56
1:B:704:ARG:CG	1:B:704:ARG:NH1	2.56	0.56
1:F:590:ARG:O	1:F:591:ASN:HB2	2.06	0.55
1:B:631:LEU:HD11	1:B:712:LEU:CD1	2.37	0.55
1:F:587:LYS:HE2	1:F:589:ARG:HG2	1.87	0.54
1:A:725:LYS:HE3	1:C:753:PHE:CE2	2.43	0.54
1:C:617:TYR:HA	2:C:1755:ATP:O1A	2.09	0.53
1:B:597:VAL:HG21	1:B:623:VAL:HG13	1.91	0.53
1:D:689:THR:HG22	4:D:2047:HOH:O	2.08	0.53
1:D:664:GLU:HG3	1:D:680:ARG:NH2	2.24	0.52
1:E:637:ARG:HH11	1:E:637:ARG:HB2	1.74	0.52
1:D:631:LEU:HD11	1:D:712:LEU:CD1	2.38	0.52
1:A:631:LEU:HD11	1:A:712:LEU:CD1	2.38	0.52
1:B:697:GLU:OE2	1:B:697:GLU:N	2.43	0.52
1:B:738:GLN:HG2	1:B:744:LEU:HD23	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:617:TYR:HA	2:E:1752:ATP:O1A	2.11	0.51
1:C:662:PHE:HB3	1:C:683:LEU:HD22	1.93	0.51
1:E:583:MET:HG2	1:E:692:ASP:O	2.11	0.51
1:A:650:LYS:HB3	1:A:652:ASP:OD1	2.10	0.51
1:E:583:MET:HB3	1:E:692:ASP:HB2	1.92	0.51
1:B:587:LYS:CD	1:B:589:ARG:HD3	2.37	0.50
1:D:667:PRO:O	1:D:669:LEU:HD22	2.11	0.50
1:D:586:MET:HE3	1:D:713:VAL:HG11	1.94	0.50
1:D:615:THR:O	1:D:637:ARG:NH2	2.44	0.50
1:B:659:ILE:HG13	1:B:669:LEU:HD21	1.93	0.50
1:B:612:ILE:O	1:B:637:ARG:NH2	2.45	0.50
1:E:622:VAL:HG11	1:E:683:LEU:HD13	1.90	0.49
1:C:598:LEU:O	1:C:622:VAL:HA	2.12	0.49
1:B:726:LYS:HG2	1:B:730:LYS:HE3	1.93	0.49
1:D:622:VAL:HG23	1:D:632:VAL:HB	1.93	0.49
1:F:700:VAL:HG22	1:F:728:VAL:HG13	1.94	0.49
1:B:630:ARG:CG	1:B:630:ARG:NH1	2.70	0.48
1:D:586:MET:CE	1:D:713:VAL:CB	2.67	0.48
1:C:704:ARG:HH22	1:C:751:VAL:HA	1.79	0.48
1:D:617:TYR:HA	2:D:1753:ATP:O1A	2.13	0.48
1:B:700:VAL:HG22	1:B:728:VAL:HG13	1.94	0.48
1:B:728:VAL:O	1:B:732:ILE:HG13	2.14	0.48
1:B:638:ARG:HD2	4:B:2021:HOH:O	2.14	0.48
1:B:698:ILE:O	1:B:702:ILE:HG13	2.13	0.48
1:E:598:LEU:HD13	1:E:603:MET:HE1	1.96	0.48
1:B:704:ARG:NH1	1:B:704:ARG:HB3	2.29	0.47
1:A:689:THR:HG22	4:A:2036:HOH:O	2.15	0.47
1:C:600:GLN:HG3	1:C:601:ASP:HB2	1.96	0.47
1:C:652:ASP:N	1:C:652:ASP:OD1	2.44	0.47
1:E:662:PHE:HB3	1:E:683:LEU:HD22	1.96	0.47
1:F:631:LEU:HD11	1:F:712:LEU:CD1	2.45	0.47
1:E:588:PRO:HD3	1:E:595:LEU:HG	1.96	0.47
1:B:704:ARG:CB	1:B:704:ARG:HH11	2.28	0.47
1:B:590:ARG:H	1:B:590:ARG:CD	2.12	0.47
1:C:598:LEU:HD22	1:C:603:MET:HE1	1.97	0.47
1:E:622:VAL:HG22	1:E:632:VAL:HB	1.97	0.46
1:C:650:LYS:CB	1:C:652:ASP:OD1	2.63	0.46
1:C:590:ARG:O	1:C:591:ASN:ND2	2.49	0.46
1:E:690:VAL:O	1:E:713:VAL:HA	2.15	0.46
1:E:608:VAL:O	1:E:612:ILE:HG13	2.15	0.46
1:D:583:MET:HB3	1:D:692:ASP:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:598:LEU:HD22	1:D:603:MET:HE1	1.98	0.46
1:F:631:LEU:HD11	1:F:712:LEU:HD13	1.98	0.46
1:D:704:ARG:NH2	1:D:751:VAL:HG13	2.31	0.46
1:D:594:LEU:HD22	1:D:594:LEU:H	1.81	0.46
1:C:615:THR:O	1:C:637:ARG:NH2	2.49	0.46
1:D:604:THR:HA	1:D:659:ILE:HA	1.98	0.46
1:C:735:MET:HA	1:C:735:MET:CE	2.46	0.45
1:C:653:GLY:HA3	1:C:675:PRO:HG3	1.98	0.45
1:F:659:ILE:HD12	1:F:669:LEU:HD21	1.97	0.45
1:C:600:GLN:HE21	1:C:632:VAL:HG21	1.82	0.45
1:C:651:GLN:CB	1:C:652:ASP:C	2.84	0.45
1:C:601:ASP:OD2	1:C:667:PRO:HB3	2.16	0.45
1:E:594:LEU:HD22	1:E:594:LEU:H	1.82	0.45
1:A:690:VAL:HG22	1:A:694:THR:OG1	2.17	0.45
1:D:588:PRO:HB2	1:D:592:ASP:HB2	1.99	0.45
1:E:670:PRO:HG2	1:E:673:THR:OG1	2.17	0.44
1:B:631:LEU:HD11	1:B:712:LEU:HD13	2.00	0.44
1:D:599:THR:OG1	1:D:603:MET:HG2	2.18	0.44
1:E:598:LEU:HD11	1:E:608:VAL:HG22	2.00	0.44
1:E:598:LEU:HD13	1:E:603:MET:CE	2.47	0.44
1:E:637:ARG:HB2	1:E:637:ARG:NH1	2.34	0.43
1:E:648:ARG:NH2	4:E:2014:HOH:O	2.51	0.43
1:D:662:PHE:HB3	1:D:683:LEU:HD22	2.01	0.43
1:F:590:ARG:O	1:F:590:ARG:HD2	2.18	0.43
1:B:615:THR:O	1:B:637:ARG:NH2	2.46	0.43
1:D:586:MET:HE3	1:D:713:VAL:CG2	2.48	0.43
1:B:592:ASP:HB3	1:B:593:PRO:HD2	2.01	0.43
1:C:612:ILE:O	1:C:637:ARG:NH2	2.51	0.43
1:B:631:LEU:HD11	1:B:712:LEU:HD12	2.00	0.43
1:E:586:MET:O	1:E:589:ARG:HD2	2.19	0.43
1:C:710:GLN:HB3	1:C:710:GLN:HE21	1.72	0.43
1:F:639:ASP:HB3	1:F:682:ILE:HG12	2.01	0.42
1:E:622:VAL:CG1	1:E:683:LEU:CD1	2.85	0.42
1:C:653:GLY:HA3	1:C:675:PRO:CG	2.49	0.42
1:B:669:LEU:HA	1:B:670:PRO:HD3	1.87	0.42
1:D:597:VAL:HG11	1:D:623:VAL:HG22	2.01	0.42
1:B:671:PRO:O	1:B:672:TYR:HB2	2.18	0.42
1:D:622:VAL:CG2	1:D:632:VAL:HB	2.49	0.42
1:E:715:HIS:O	1:E:718:ARG:HB3	2.20	0.42
1:B:688:PHE:CE2	1:B:702:ILE:HG21	2.54	0.42
1:C:670:PRO:HA	1:C:671:PRO:HD3	1.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:THR:HG22	1:D:659:ILE:HG12	2.02	0.41
1:C:644:ILE:O	1:C:648:ARG:CG	2.63	0.41
1:E:631:LEU:HD23	1:E:719:LEU:HD22	2.02	0.41
1:D:609:GLU:CD	1:D:648:ARG:NH1	2.74	0.41
1:B:747:GLU:O	1:B:750:GLU:HB2	2.21	0.41
1:E:598:LEU:CD1	1:E:608:VAL:HG22	2.51	0.41
1:D:598:LEU:CD2	1:D:603:MET:HE1	2.50	0.41
1:A:632:VAL:HG12	1:A:683:LEU:HD21	2.02	0.41
1:F:589:ARG:NE	1:F:589:ARG:HA	2.35	0.41
1:C:704:ARG:NH2	1:C:751:VAL:HG13	2.35	0.41
1:A:600:GLN:HE21	1:A:632:VAL:HG21	1.86	0.41
1:B:579:LYS:HD3	1:B:695:PRO:HB3	2.03	0.40
1:C:580:THR:HG23	1:C:696:MET:HB2	2.04	0.40
1:F:689:THR:CG2	1:F:690:VAL:N	2.84	0.40
1:B:590:ARG:N	1:B:590:ARG:HD3	2.25	0.40
1:E:652:ASP:OD1	1:E:652:ASP:N	2.54	0.40
1:E:615:THR:O	1:E:637:ARG:NH2	2.55	0.40
1:A:628:SER:HA	1:A:718:ARG:HH11	1.85	0.40
1:B:600:GLN:NE2	1:B:632:VAL:HG21	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1755:CL:CL	3:D:1755:CL:CL[2_665]	0.94	1.26

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	163/185 (88%)	154 (94%)	8 (5%)	1 (1%)	30 36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	167/185 (90%)	163 (98%)	4 (2%)	0	100	100
1	C	168/185 (91%)	162 (96%)	5 (3%)	1 (1%)	30	36
1	D	167/185 (90%)	164 (98%)	3 (2%)	0	100	100
1	E	163/185 (88%)	159 (98%)	4 (2%)	0	100	100
1	F	156/185 (84%)	148 (95%)	8 (5%)	0	100	100
All	All	984/1110 (89%)	950 (96%)	32 (3%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	652	ASP
1	A	671	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	156/173 (90%)	146 (94%)	10 (6%)	22	28
1	B	160/173 (92%)	151 (94%)	9 (6%)	26	35
1	C	161/173 (93%)	144 (89%)	17 (11%)	8	9
1	D	158/173 (91%)	148 (94%)	10 (6%)	22	29
1	E	156/173 (90%)	145 (93%)	11 (7%)	18	23
1	F	146/173 (84%)	138 (94%)	8 (6%)	27	36
All	All	937/1038 (90%)	872 (93%)	65 (7%)	19	24

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	595	LEU
1	A	631	LEU
1	A	637	ARG
1	A	638	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	650	LYS
1	A	652	ASP
1	A	669	LEU
1	A	677	LEU
1	A	680	ARG
1	A	746	ASN
1	B	590	ARG
1	B	601	ASP
1	B	630	ARG
1	B	631	LEU
1	B	677	LEU
1	B	690	VAL
1	B	697	GLU
1	B	704	ARG
1	B	710	GLN
1	C	580	THR
1	C	587	LYS
1	C	591	ASN
1	C	595	LEU
1	C	601	ASP
1	C	610	THR
1	C	631	LEU
1	C	637	ARG
1	C	650	LYS
1	C	652	ASP
1	C	669	LEU
1	C	677	LEU
1	C	690	VAL
1	C	710	GLN
1	C	720	LEU
1	C	735	MET
1	C	738	GLN
1	D	622	VAL
1	D	631	LEU
1	D	654	VAL
1	D	677	LEU
1	D	680	ARG
1	D	690	VAL
1	D	710	GLN
1	D	718	ARG
1	D	720	LEU
1	D	738	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	590	ARG
1	E	622	VAL
1	E	630	ARG
1	E	650	LYS
1	E	656	SER
1	E	669	LEU
1	E	677	LEU
1	E	690	VAL
1	E	710	GLN
1	E	718	ARG
1	E	746	ASN
1	F	580	THR
1	F	587	LYS
1	F	590	ARG
1	F	631	LEU
1	F	680	ARG
1	F	690	VAL
1	F	710	GLN
1	F	720	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	GLN
1	A	746	ASN
1	B	600	GLN
1	B	734	GLN
1	B	737	ASN
1	B	738	GLN
1	C	591	ASN
1	C	600	GLN
1	C	646	ASN
1	C	710	GLN
1	C	731	HIS
1	C	734	GLN
1	C	738	GLN
1	D	600	GLN
1	D	710	GLN
1	D	738	GLN
1	E	591	ASN
1	E	600	GLN
1	E	737	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	600	GLN
1	F	731	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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	ATP	A	1752	-	24,33,33	1.40	3 (12%)	31,52,52	2.20	5 (16%)
2	ATP	B	1754	-	24,33,33	1.33	3 (12%)	31,52,52	2.21	3 (9%)
2	ATP	C	1755	-	24,33,33	1.36	3 (12%)	31,52,52	2.06	4 (12%)
2	ATP	D	1753	-	24,33,33	1.43	3 (12%)	31,52,52	2.19	4 (12%)
2	ATP	E	1752	-	24,33,33	1.32	3 (12%)	31,52,52	2.24	5 (16%)
2	ATP	F	1750	-	24,33,33	1.25	3 (12%)	31,52,52	2.27	6 (19%)

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	ATP	A	1752	-	-	0/18/38/38	0/3/3/3
2	ATP	B	1754	-	-	0/18/38/38	0/3/3/3
2	ATP	C	1755	-	-	0/18/38/38	0/3/3/3
2	ATP	D	1753	-	-	0/18/38/38	0/3/3/3
2	ATP	E	1752	-	-	0/18/38/38	0/3/3/3
2	ATP	F	1750	-	-	0/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1755	ATP	PG-O2G	2.04	1.62	1.54
2	F	1750	ATP	O4'-C1'	2.12	1.43	1.41
2	F	1750	ATP	PG-O2G	2.21	1.62	1.54
2	E	1752	ATP	PG-O2G	2.36	1.63	1.54
2	B	1754	ATP	PG-O2G	2.41	1.63	1.54
2	E	1752	ATP	O4'-C1'	2.45	1.44	1.41
2	A	1752	ATP	PG-O2G	2.49	1.63	1.54
2	D	1753	ATP	O4'-C1'	2.57	1.44	1.41
2	A	1752	ATP	O4'-C1'	2.60	1.44	1.41
2	B	1754	ATP	O4'-C1'	2.61	1.44	1.41
2	C	1755	ATP	O4'-C1'	2.62	1.44	1.41
2	D	1753	ATP	PG-O2G	2.79	1.64	1.54
2	B	1754	ATP	PG-O1G	3.27	1.61	1.51
2	C	1755	ATP	PG-O1G	3.53	1.62	1.51
2	F	1750	ATP	PG-O1G	3.58	1.63	1.51
2	E	1752	ATP	PG-O1G	3.78	1.63	1.51
2	D	1753	ATP	PG-O1G	3.80	1.63	1.51
2	A	1752	ATP	PG-O1G	3.88	1.63	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1753	ATP	N3-C2-N1	-9.91	121.31	128.89
2	A	1752	ATP	N3-C2-N1	-9.70	121.47	128.89
2	B	1754	ATP	N3-C2-N1	-9.66	121.50	128.89
2	E	1752	ATP	N3-C2-N1	-9.58	121.56	128.89
2	F	1750	ATP	N3-C2-N1	-9.42	121.68	128.89
2	C	1755	ATP	N3-C2-N1	-9.03	121.98	128.89
2	B	1754	ATP	PB-O3B-PG	-4.19	118.60	132.67
2	F	1750	ATP	PA-O3A-PB	-4.13	121.13	132.73
2	E	1752	ATP	PB-O3B-PG	-4.09	118.96	132.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1753	ATP	PB-O3B-PG	-3.70	120.27	132.67
2	E	1752	ATP	C2'-C1'-N9	-3.49	108.96	114.29
2	F	1750	ATP	PB-O3B-PG	-3.44	121.13	132.67
2	A	1752	ATP	PA-O3A-PB	-3.42	123.13	132.73
2	B	1754	ATP	C2'-C1'-N9	-3.37	109.14	114.29
2	C	1755	ATP	PB-O3B-PG	-3.34	121.46	132.67
2	A	1752	ATP	PB-O3B-PG	-3.31	121.55	132.67
2	E	1752	ATP	PA-O3A-PB	-3.11	124.00	132.73
2	A	1752	ATP	C2'-C1'-N9	-3.06	109.61	114.29
2	C	1755	ATP	C4-C5-N7	-3.02	106.70	109.48
2	F	1750	ATP	C2'-C1'-N9	-2.77	110.06	114.29
2	D	1753	ATP	PA-O3A-PB	-2.33	126.18	132.73
2	F	1750	ATP	C5'-C4'-C3'	-2.25	106.30	115.21
2	E	1752	ATP	C4-C5-N7	-2.10	107.55	109.48
2	F	1750	ATP	C4-C5-N7	-2.03	107.61	109.48
2	A	1752	ATP	C4-C5-N7	-2.01	107.63	109.48
2	D	1753	ATP	C4-C5-N7	-2.00	107.64	109.48
2	C	1755	ATP	O3G-PG-O3B	2.37	115.86	105.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1752	ATP	1	0
2	C	1755	ATP	1	0
2	D	1753	ATP	1	0
2	E	1752	ATP	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	167/185 (90%)	0.98	30 (17%) 2 3	18, 25, 39, 93	0
1	B	171/185 (92%)	0.70	20 (11%) 6 10	16, 23, 39, 42	0
1	C	172/185 (92%)	0.67	15 (8%) 13 18	18, 23, 34, 41	0
1	D	171/185 (92%)	0.70	21 (12%) 5 8	18, 23, 37, 81	0
1	E	167/185 (90%)	0.97	29 (17%) 2 3	21, 27, 47, 51	0
1	F	162/185 (87%)	2.67	87 (53%) 0 0	29, 72, 132, 139	0
All	All	1010/1110 (90%)	1.10	202 (20%) 1 2	16, 26, 97, 139	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	662	PHE	14.0
1	F	660	ILE	11.0
1	F	672	TYR	10.6
1	F	671	PRO	9.6
1	E	651	GLN	9.5
1	F	598	LEU	8.3
1	B	672	TYR	7.7
1	F	659	ILE	7.5
1	F	669	LEU	7.1
1	F	749	LEU	7.0
1	C	590	ARG	6.9
1	F	597	VAL	6.8
1	F	638	ARG	6.6
1	F	641	ILE	6.5
1	A	651	GLN	6.1
1	F	649	LYS	5.9
1	E	649	LYS	5.9
1	A	672	TYR	5.9
1	C	744	LEU	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	595	LEU	5.7
1	F	620	PHE	5.5
1	F	617	TYR	5.2
1	E	642	ILE	5.2
1	E	591	ASN	5.1
1	F	665	HIS	5.1
1	E	652	ASP	5.1
1	E	654	VAL	5.0
1	F	663	THR	5.0
1	A	745	PHE	5.0
1	F	578	HIS	5.0
1	F	605	VAL	5.0
1	F	722	ILE	4.9
1	F	644	ILE	4.9
1	B	579	LYS	4.9
1	F	600	GLN	4.7
1	A	671	PRO	4.6
1	F	603	MET	4.6
1	F	585	VAL	4.6
1	A	650	LYS	4.5
1	B	744	LEU	4.5
1	F	743	ILE	4.4
1	D	748	PHE	4.4
1	E	648	ARG	4.4
1	F	596	THR	4.3
1	F	688	PHE	4.3
1	F	661	TYR	4.3
1	A	595	LEU	4.3
1	A	749	LEU	4.3
1	F	599	THR	4.2
1	A	751	VAL	4.2
1	F	655	VAL	4.2
1	F	677	LEU	4.2
1	F	723	ILE	4.1
1	E	709	ARG	4.0
1	F	640	LEU	4.0
1	C	651	GLN	4.0
1	F	616	THR	4.0
1	A	748	PHE	4.0
1	D	672	TYR	4.0
1	F	622	VAL	3.9
1	F	664	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	586	MET	3.9
1	F	591	ASN	3.9
1	F	657	THR	3.9
1	D	590	ARG	3.9
1	F	679	LEU	3.8
1	F	731	HIS	3.8
1	C	591	ASN	3.8
1	C	754	GLN	3.8
1	F	748	PHE	3.7
1	F	746	ASN	3.7
1	B	738	GLN	3.6
1	F	643	SER	3.6
1	A	578	HIS	3.6
1	F	728	VAL	3.6
1	F	729	LEU	3.6
1	F	675	PRO	3.5
1	D	665	HIS	3.5
1	F	709	ARG	3.5
1	F	745	PHE	3.5
1	A	590	ARG	3.4
1	B	651	GLN	3.4
1	D	752	LEU	3.4
1	E	592	ASP	3.4
1	D	578	HIS	3.4
1	F	727	ASP	3.4
1	E	655	VAL	3.4
1	F	621	PRO	3.4
1	E	614	GLU	3.4
1	F	658	SER	3.4
1	F	608	VAL	3.3
1	F	619	GLY	3.3
1	F	592	ASP	3.2
1	E	638	ARG	3.2
1	F	604	THR	3.2
1	F	627	GLU	3.1
1	F	676	THR	3.1
1	A	746	ASN	3.1
1	D	627	GLU	3.1
1	F	678	LYS	3.1
1	F	668	PRO	3.0
1	C	749	LEU	3.0
1	D	746	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	595	LEU	3.0
1	A	670	PRO	3.0
1	E	590	ARG	3.0
1	A	709	ARG	3.0
1	A	627	GLU	3.0
1	B	660	ILE	2.9
1	B	669	LEU	2.9
1	A	635	VAL	2.9
1	F	618	SER	2.9
1	D	641	ILE	2.9
1	F	642	ILE	2.9
1	A	750	GLU	2.8
1	F	606	GLU	2.8
1	F	654	VAL	2.8
1	F	734	GLN	2.8
1	E	671	PRO	2.8
1	B	712	LEU	2.8
1	F	587	LYS	2.8
1	A	747	GLU	2.8
1	E	723	ILE	2.8
1	B	671	PRO	2.8
1	D	638	ARG	2.7
1	F	697	GLU	2.7
1	F	579	LYS	2.7
1	D	709	ARG	2.7
1	D	579	LYS	2.7
1	F	670	PRO	2.7
1	F	624	VAL	2.7
1	D	749	LEU	2.7
1	A	652	ASP	2.7
1	C	652	ASP	2.7
1	F	653	GLY	2.6
1	B	736	ALA	2.6
1	F	593	PRO	2.6
1	F	648	ARG	2.6
1	F	582	ALA	2.6
1	E	633	GLY	2.6
1	F	602	SER	2.6
1	E	627	GLU	2.6
1	B	590	ARG	2.6
1	D	591	ASN	2.6
1	B	578	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	753	PHE	2.5
1	D	745	PHE	2.5
1	E	737	ASN	2.5
1	B	640	LEU	2.5
1	C	752	LEU	2.5
1	F	613	SER	2.5
1	D	662	PHE	2.5
1	A	638	ARG	2.5
1	B	747	GLU	2.5
1	D	660	ILE	2.4
1	A	649	LYS	2.4
1	A	645	GLU	2.4
1	B	652	ASP	2.4
1	D	699	VAL	2.4
1	C	716	ASN	2.4
1	F	589	ARG	2.4
1	B	713	VAL	2.4
1	A	620	PHE	2.4
1	E	650	LYS	2.4
1	E	746	ASN	2.3
1	F	681	ASN	2.3
1	A	584	ASP	2.3
1	E	736	ALA	2.3
1	E	646	ASN	2.3
1	C	735	MET	2.3
1	F	628	SER	2.3
1	A	594	LEU	2.3
1	E	598	LEU	2.3
1	F	680	ARG	2.3
1	A	597	VAL	2.3
1	C	746	ASN	2.3
1	F	630	ARG	2.3
1	F	732	ILE	2.2
1	F	666	SER	2.2
1	E	718	ARG	2.2
1	F	581	LEU	2.2
1	A	673	THR	2.2
1	C	592	ASP	2.2
1	D	650	LYS	2.2
1	E	699	VAL	2.2
1	B	709	ARG	2.2
1	A	621	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	660	ILE	2.1
1	F	712	LEU	2.1
1	A	644	ILE	2.1
1	C	712	LEU	2.1
1	A	648	ARG	2.1
1	E	610	THR	2.1
1	B	608	VAL	2.1
1	F	632	VAL	2.1
1	B	711	CYS	2.1
1	D	621	PRO	2.1
1	B	627	GLU	2.1
1	E	745	PHE	2.0
1	F	639	ASP	2.0
1	D	652	ASP	2.0
1	E	640	LEU	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. 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(\AA^2)	Q<0.9
2	ATP	B	1754	31/31	0.86	0.17	-0.19	44,48,61,62	0
2	ATP	E	1752	31/31	0.88	0.14	-0.71	65,66,71,71	0
2	ATP	D	1753	31/31	0.87	0.13	-0.72	42,44,58,58	0
2	ATP	C	1755	31/31	0.88	0.15	-0.77	41,45,58,58	0
2	ATP	A	1752	31/31	0.88	0.14	-0.89	49,51,61,62	0
2	ATP	F	1750	31/31	0.82	0.19	-2.46	95,95,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	B	3002	1/1	0.97	0.07	-	64,64,64,64	0
3	CL	E	1753	1/1	0.96	0.09	-	99,99,99,99	0
3	CL	D	1754	1/1	0.78	0.20	-	83,83,83,83	0
3	CL	C	1756	1/1	0.81	0.14	-	124,124,124,124	0
3	CL	F	3001	1/1	0.78	0.20	-	80,80,80,80	0
3	CL	B	3001	1/1	0.95	0.14	-	68,68,68,68	0
3	CL	D	3001	1/1	0.98	0.19	-	70,70,70,70	0
3	CL	F	1751	1/1	0.88	0.18	-	108,108,108,108	0
3	CL	A	1753	1/1	0.60	0.12	-	87,87,87,87	0
3	CL	D	1755	1/1	0.98	0.10	-	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.