W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:15 PM GMT

PDB ID	:	5C1B
Title	:	p97-delta709-728 in complex with a UFD1-SHP peptide
Authors	:	Haenzelmann, P.; Schindelin, H.
Deposited on	:	2015-06-13
Resolution	:	3.08 Å(reported)

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

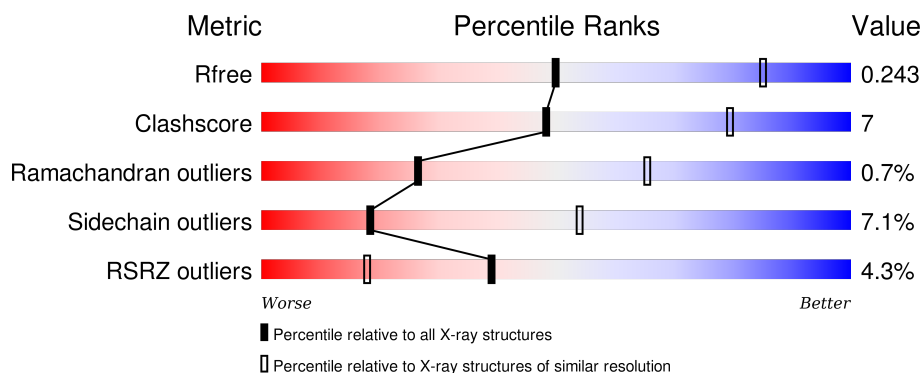|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.08 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	Percentile Ranks	Value
Rfree		0.243
Clashscore		7
Ramachandran outliers		0.7%
Sidechain outliers		7.1%
RSRZ outliers		4.3%

Worse   *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

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 <=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	785	4% / 70% 19% • 8%
1	B	785	2% / 74% 16% • 8%
1	C	785	2% / 75% 14% • 8%
1	D	785	4% / 74% 16% • 8%
1	E	785	2% / 74% 16% • 8%

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Mol	Chain	Length	Quality of chain
1	F	785	9% 75% 16% 8%
2	U	21	10% 24% 24% 52%
2	V	21	5% 24% 29% 48%

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
6	GOL	F	906	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 69385 atoms, of which 34726 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	724	Total 11417	C 3572	H 5739	N 1003	O 1073	S 30	0	0	0
1	B	724	Total 11426	C 3572	H 5748	N 1003	O 1073	S 30	0	0	0
1	C	724	Total 11427	C 3572	H 5749	N 1003	O 1073	S 30	0	0	0
1	D	724	Total 11427	C 3572	H 5749	N 1003	O 1073	S 30	0	0	0
1	E	724	Total 11426	C 3572	H 5748	N 1003	O 1073	S 30	0	0	0
1	F	724	Total 11427	C 3572	H 5749	N 1003	O 1073	S 30	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	ARG	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	ARG	deletion	UNP P55072
A	?	-	GLN	deletion	UNP P55072
A	?	-	THR	deletion	UNP P55072
A	?	-	ASN	deletion	UNP P55072
A	?	-	PRO	deletion	UNP P55072
A	?	-	SER	deletion	UNP P55072
A	?	-	ALA	deletion	UNP P55072
A	?	-	MET	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	VAL	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	ASP	deletion	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P55072
A	?	-	PRO	deletion	UNP P55072
A	?	-	VAL	deletion	UNP P55072
B	?	-	ARG	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	ARG	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	ARG	deletion	UNP P55072
B	?	-	GLN	deletion	UNP P55072
B	?	-	THR	deletion	UNP P55072
B	?	-	ASN	deletion	UNP P55072
B	?	-	PRO	deletion	UNP P55072
B	?	-	SER	deletion	UNP P55072
B	?	-	ALA	deletion	UNP P55072
B	?	-	MET	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	VAL	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	ASP	deletion	UNP P55072
B	?	-	ASP	deletion	UNP P55072
B	?	-	PRO	deletion	UNP P55072
B	?	-	VAL	deletion	UNP P55072
C	?	-	ARG	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	ARG	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	ARG	deletion	UNP P55072
C	?	-	GLN	deletion	UNP P55072
C	?	-	THR	deletion	UNP P55072
C	?	-	ASN	deletion	UNP P55072
C	?	-	PRO	deletion	UNP P55072
C	?	-	SER	deletion	UNP P55072
C	?	-	ALA	deletion	UNP P55072
C	?	-	MET	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	VAL	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	ASP	deletion	UNP P55072
C	?	-	ASP	deletion	UNP P55072
C	?	-	PRO	deletion	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP P55072
D	?	-	ARG	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	ARG	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	ARG	deletion	UNP P55072
D	?	-	GLN	deletion	UNP P55072
D	?	-	THR	deletion	UNP P55072
D	?	-	ASN	deletion	UNP P55072
D	?	-	PRO	deletion	UNP P55072
D	?	-	SER	deletion	UNP P55072
D	?	-	ALA	deletion	UNP P55072
D	?	-	MET	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	VAL	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	ASP	deletion	UNP P55072
D	?	-	ASP	deletion	UNP P55072
D	?	-	PRO	deletion	UNP P55072
D	?	-	VAL	deletion	UNP P55072
E	?	-	ARG	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	ARG	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	ARG	deletion	UNP P55072
E	?	-	GLN	deletion	UNP P55072
E	?	-	THR	deletion	UNP P55072
E	?	-	ASN	deletion	UNP P55072
E	?	-	PRO	deletion	UNP P55072
E	?	-	SER	deletion	UNP P55072
E	?	-	ALA	deletion	UNP P55072
E	?	-	MET	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	VAL	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	ASP	deletion	UNP P55072
E	?	-	ASP	deletion	UNP P55072
E	?	-	PRO	deletion	UNP P55072
E	?	-	VAL	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLU	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072
F	?	-	GLN	deletion	UNP P55072
F	?	-	THR	deletion	UNP P55072
F	?	-	ASN	deletion	UNP P55072
F	?	-	PRO	deletion	UNP P55072
F	?	-	SER	deletion	UNP P55072
F	?	-	ALA	deletion	UNP P55072
F	?	-	MET	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	VAL	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	ASP	deletion	UNP P55072
F	?	-	ASP	deletion	UNP P55072
F	?	-	PRO	deletion	UNP P55072
F	?	-	VAL	deletion	UNP P55072

- Molecule 2 is a protein called Ubiquitin fusion degradation protein 1 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	11	Total 125	C 53	H 40	N 18	O 14	0	0	0
2	U	10	Total 106	C 44	H 32	N 17	O 13	0	0	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).
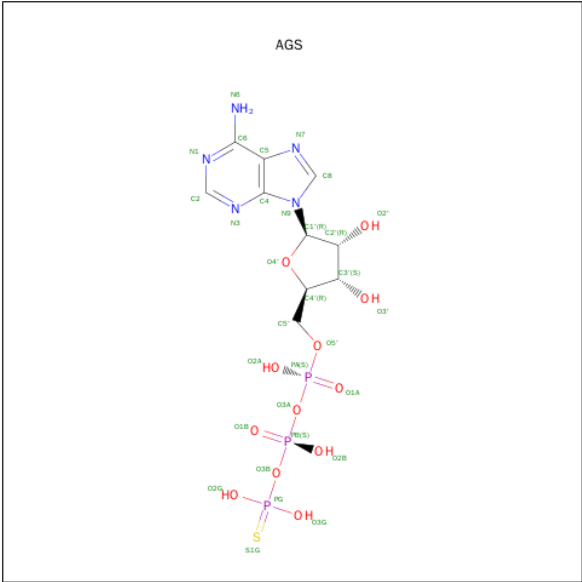
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	E	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	E	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total 2	Mg 2	0	0
4	E	2	Total 2	Mg 2	0	0
4	B	2	Total 2	Mg 2	0	0
4	C	2	Total 2	Mg 2	0	0
4	A	2	Total 2	Mg 2	0	0
4	F	2	Total 2	Mg 2	0	0

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

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total 14	C 3	H 8	O 3	0	0
6	F	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 7 is water.

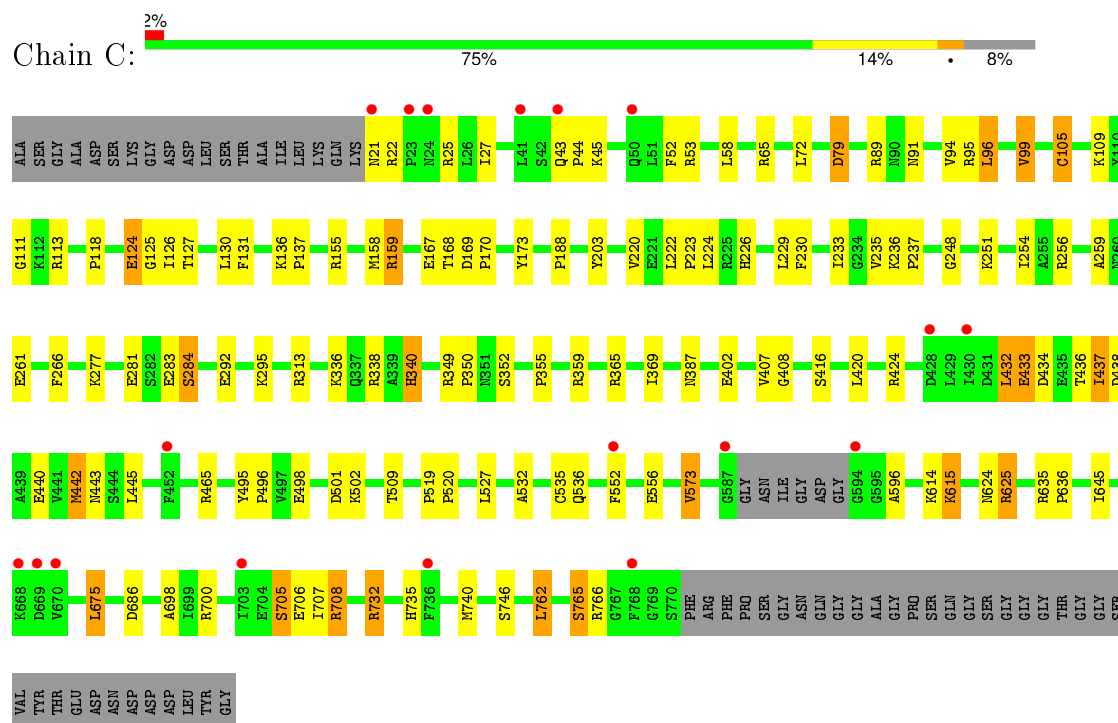| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total 5	O 5	0	0
7	B	5	Total 5	O 5	0	0
7	C	5	Total 5	O 5	0	0
7	D	5	Total 5	O 5	0	0
7	E	5	Total 5	O 5	0	0
7	F	5	Total 5	O 5	0	0

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.
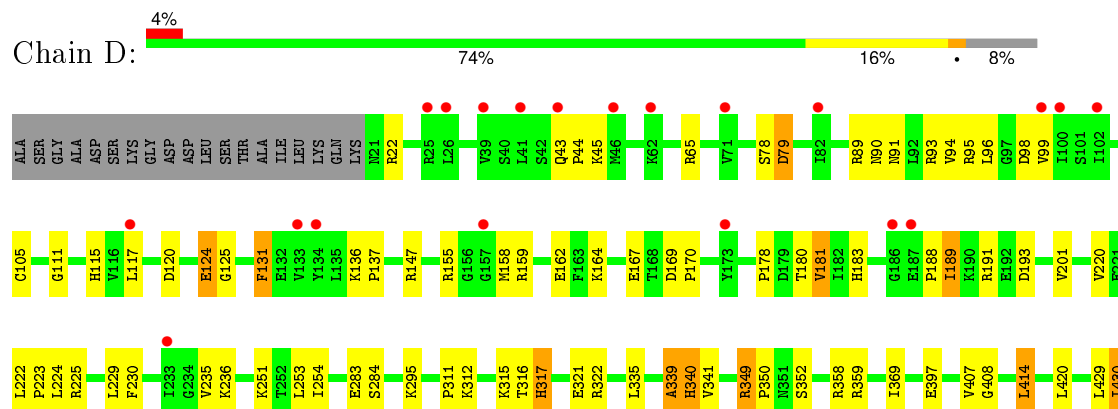
- Molecule 1: Transitional endoplasmic reticulum ATPase

- Molecule 1: Transitional endoplasmic reticulum ATPase

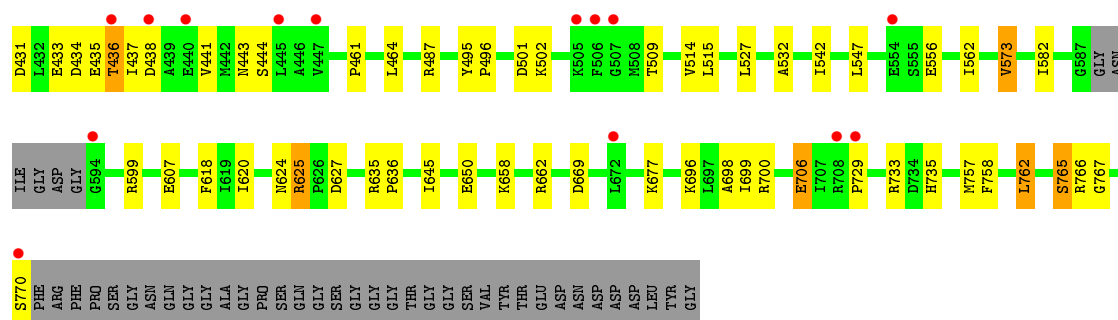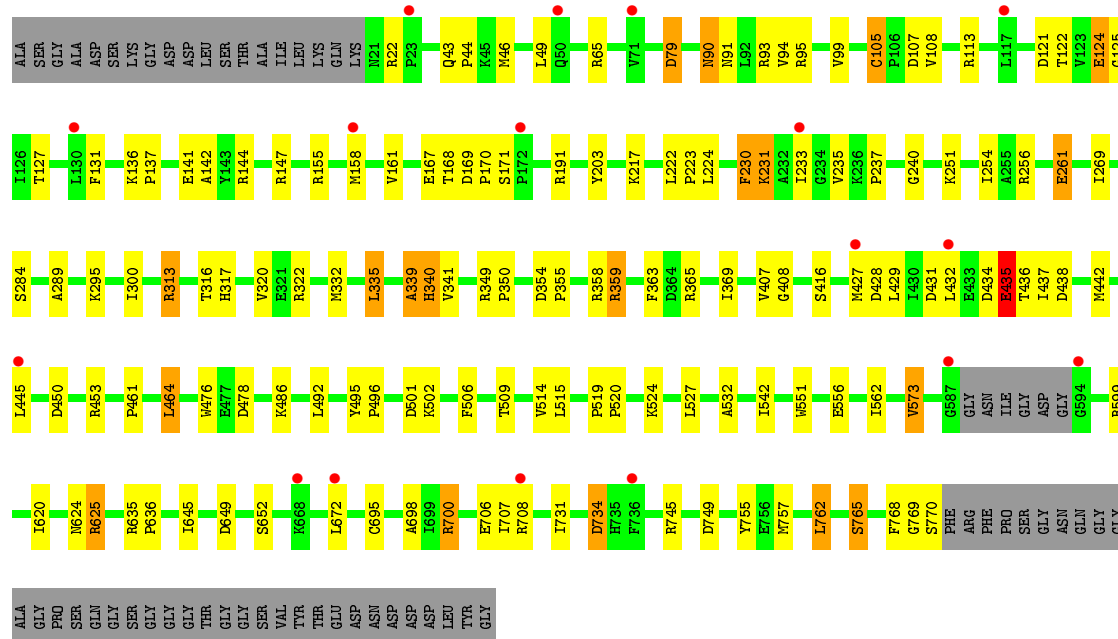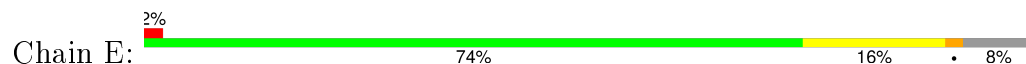• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:

• Molecule 1: Transitional endoplasmic reticulum ATPase

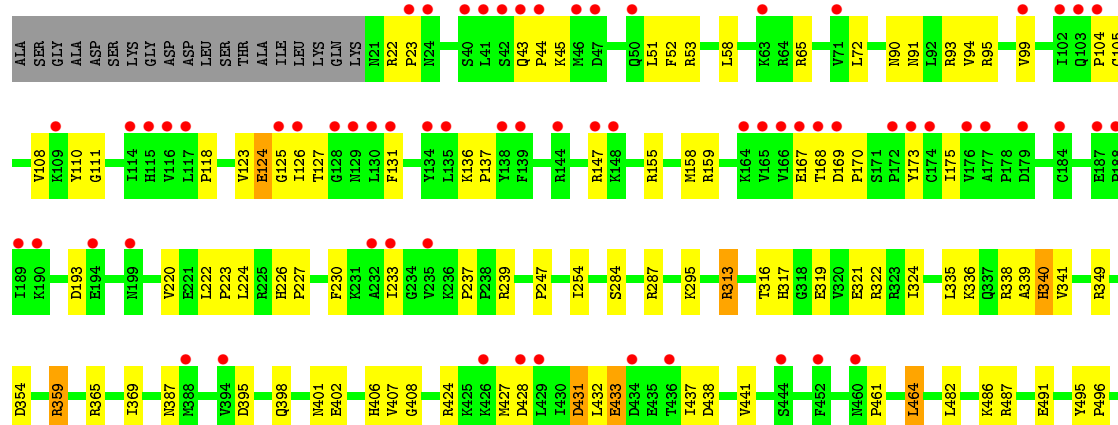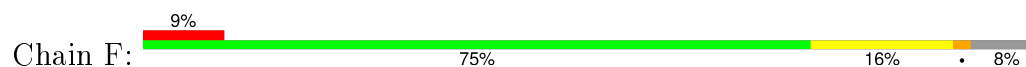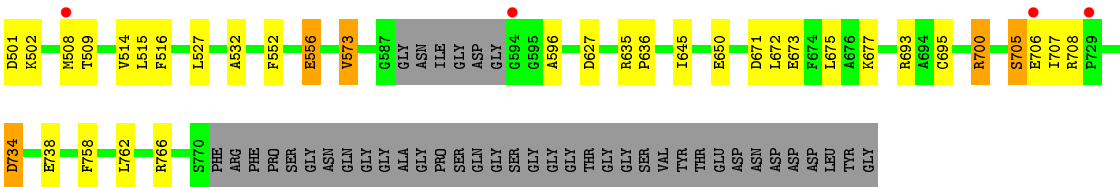Chain D:

• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:

• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:

• Molecule 2: Ubiquitin fusion degradation protein 1 homolog

Chain V:

• Molecule 2: Ubiquitin fusion degradation protein 1 homolog

Chain U:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	140.72Å　　180.66Å　　254.96Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	49.14　–　3.08 49.14　–　3.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.14-3.08) 100.0 (49.14-3.08)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198　,　0.240 0.204　,　0.243	Depositor DCC
R_{free} test set	6055 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	108.5	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 85.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 120506 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	69385	wwPDB-VP
Average B, all atoms (Å^2)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, MG, AGS, 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	0.22	0/5771	0.44	0/7791
1	B	0.22	0/5771	0.43	0/7791
1	C	0.22	0/5771	0.44	0/7791
1	D	0.23	0/5771	0.44	0/7791
1	E	0.22	0/5771	0.42	0/7791
1	F	0.22	0/5771	0.44	0/7791
2	U	0.25	0/74	0.51	0/96
2	V	0.26	0/86	0.56	0/112
All	All	0.22	0/34786	0.44	0/46954

There are no bond length outliers.

There are no bond angle outliers.

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	5678	5739	5749	107	1
1	B	5678	5748	5749	84	0
1	C	5678	5749	5749	74	1
1	D	5678	5749	5749	88	1
1	E	5678	5748	5749	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5678	5749	5749	74	1
2	U	74	32	72	17	0
2	V	85	40	81	22	0
3	A	62	26	24	4	0
3	B	62	26	24	1	0
3	C	62	26	24	3	0
3	D	62	26	24	1	0
3	E	62	26	24	4	0
3	F	62	26	24	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	F	12	16	16	0	0
7	A	5	0	0	1	0
7	B	5	0	0	2	0
7	C	5	0	0	1	0
7	D	5	0	0	0	0
7	E	5	0	0	1	0
7	F	5	0	0	1	0
All	All	34659	34726	34807	510	2

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 7.

All (510) 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:162:GLU:OE1	1:A:191:ARG:NH2	1.83	1.10
2:V:227:ALA:HB1	2:V:228:PHE:CD1	2.02	0.94
1:D:162:GLU:OE1	1:D:191:ARG:NH2	2.04	0.91
1:B:429:LEU:O	1:B:431:ASP:N	2.04	0.90
1:D:181:VAL:HA	2:V:233:ASN:HB3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:227:ALA:HB1	2:U:228:PHE:CD1	2.08	0.87
1:E:339:ALA:O	1:E:341:VAL:N	2.10	0.84
1:A:321:GLU:OE2	1:B:322:ARG:NH2	2.10	0.83
1:A:766:ARG:NH1	3:F:902:AGS:S1G	2.52	0.82
1:D:65:ARG:NH1	1:D:91:ASN:O	2.12	0.81
1:A:181:VAL:HA	2:U:233:ASN:HB3	1.60	0.81
3:F:901:AGS:O1A	7:F:1001:HOH:O	1.98	0.80
1:B:304:ASP:OD2	7:B:1001:HOH:O	1.99	0.79
1:C:65:ARG:NH1	1:C:91:ASN:O	2.15	0.79
3:A:901:AGS:O3G	7:A:1001:HOH:O	2.00	0.79
1:D:339:ALA:O	1:D:341:VAL:N	2.15	0.79
1:E:65:ARG:NH1	1:E:91:ASN:O	2.16	0.79
1:C:251:LYS:NZ	3:C:902:AGS:O1B	2.18	0.77
1:A:434:ASP:OD2	1:B:226:HIS:ND1	2.19	0.76
1:A:339:ALA:O	1:A:341:VAL:N	2.22	0.73
1:D:251:LYS:NZ	3:D:902:AGS:O1B	2.22	0.73
1:B:304:ASP:OD1	7:B:1002:HOH:O	2.06	0.72
1:E:434:ASP:O	1:E:435:GLU:HG2	1.88	0.72
1:A:178:PRO:HA	2:U:235:LEU:HD13	1.71	0.72
1:E:124:GLU:OE1	1:E:125:GLY:N	2.23	0.72
3:E:901:AGS:O1A	7:E:1001:HOH:O	2.08	0.71
1:A:79:ASP:N	1:A:79:ASP:OD1	2.24	0.71
1:D:79:ASP:OD1	1:D:79:ASP:N	2.24	0.70
1:D:321:GLU:OE2	1:E:322:ARG:NH2	2.24	0.70
1:B:65:ARG:NH1	1:B:91:ASN:O	2.25	0.69
1:D:650:GLU:OE1	1:D:677:LYS:HG3	1.93	0.69
2:U:232:GLY:O	2:U:234:ARG:N	2.24	0.69
2:V:233:ASN:OD1	2:V:234:ARG:N	2.25	0.68
1:E:79:ASP:N	1:E:79:ASP:OD1	2.27	0.68
1:E:434:ASP:O	1:E:435:GLU:CG	2.42	0.67
1:C:79:ASP:N	1:C:79:ASP:OD1	2.27	0.67
2:V:232:GLY:O	2:V:234:ARG:N	2.26	0.67
1:D:178:PRO:HA	2:V:235:LEU:HD13	1.77	0.66
1:F:65:ARG:NH1	1:F:91:ASN:O	2.29	0.66
1:A:65:ARG:NH1	1:A:91:ASN:O	2.28	0.66
2:U:233:ASN:OD1	2:U:234:ARG:N	2.27	0.66
1:E:700:ARG:NH1	1:F:491:GLU:OE2	2.29	0.65
1:F:734:ASP:OD1	1:F:734:ASP:N	2.28	0.65
1:D:131:PHE:CE2	2:V:234:ARG:NH1	2.65	0.65
2:V:227:ALA:HB1	2:V:228:PHE:CE1	2.31	0.65
1:F:339:ALA:O	1:F:341:VAL:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:LEU:HD11	1:F:226:HIS:CG	2.32	0.64
1:A:339:ALA:O	1:A:341:VAL:HG23	1.97	0.64
2:V:228:PHE:O	2:V:229:SER:HB3	1.98	0.64
1:C:113:ARG:NH1	1:C:169:ASP:OD1	2.31	0.63
1:A:115:HIS:NE2	2:U:227:ALA:O	2.32	0.62
1:E:158:MET:HE1	1:E:445:LEU:HD13	1.81	0.62
2:U:228:PHE:O	2:U:229:SER:HB3	1.99	0.62
2:V:226:ARG:HG3	2:V:227:ALA:N	2.15	0.61
1:A:251:LYS:NZ	3:A:901:AGS:O1B	2.33	0.61
1:A:158:MET:CE	1:B:235:VAL:HG21	2.30	0.61
1:E:339:ALA:O	1:E:341:VAL:HG23	2.00	0.61
1:E:434:ASP:OD2	1:E:437:ILE:HD13	2.00	0.61
1:D:222:LEU:HB2	1:D:223:PRO:HD3	1.83	0.60
1:E:169:ASP:HB3	1:E:170:PRO:HD3	1.82	0.60
1:E:43:GLN:N	1:E:44:PRO:HD2	2.16	0.60
1:B:43:GLN:N	1:B:44:PRO:HD2	2.16	0.59
2:V:228:PHE:O	2:V:229:SER:CB	2.50	0.59
1:F:43:GLN:N	1:F:44:PRO:HD2	2.17	0.59
1:D:339:ALA:O	1:D:341:VAL:HG23	2.02	0.59
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.85	0.59
1:A:231:LYS:HD3	1:A:232:ALA:N	2.16	0.59
1:C:43:GLN:N	1:C:44:PRO:HD2	2.17	0.59
1:E:90:ASN:O	1:E:93:ARG:NH1	2.35	0.59
1:B:142:ALA:HB1	1:B:144:ARG:HG3	1.84	0.58
1:A:222:LEU:HB2	1:A:223:PRO:HD3	1.84	0.58
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.86	0.58
2:U:228:PHE:O	2:U:229:SER:CB	2.52	0.58
1:B:162:GLU:OE1	1:B:191:ARG:NH2	2.36	0.58
1:A:247:PRO:HB3	3:A:901:AGS:S1G	2.44	0.57
1:B:79:ASP:OD1	1:B:79:ASP:N	2.37	0.57
1:D:43:GLN:N	1:D:44:PRO:HD2	2.20	0.57
1:B:350:PRO:O	1:B:358:ARG:NH2	2.38	0.57
1:A:43:GLN:N	1:A:44:PRO:HD2	2.19	0.57
1:B:461:PRO:HG2	1:B:464:LEU:HD21	1.87	0.57
1:F:169:ASP:HB3	1:F:170:PRO:HD3	1.87	0.57
1:B:427:MET:O	1:B:428:ASP:C	2.43	0.57
1:C:338:ARG:CG	1:C:338:ARG:O	2.52	0.57
1:A:96:LEU:O	1:A:225:ARG:NH2	2.38	0.57
1:B:339:ALA:O	1:B:341:VAL:N	2.35	0.56
1:D:169:ASP:HB3	1:D:170:PRO:HD3	1.87	0.56
1:C:220:VAL:CG1	1:C:224:LEU:HD12	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.86	0.56
1:B:230:PHE:HA	1:B:233:ILE:HG22	1.88	0.56
2:U:227:ALA:HB1	2:U:228:PHE:CE1	2.39	0.56
1:A:678:MET:HA	1:A:678:MET:CE	2.36	0.56
1:D:90:ASN:O	1:D:93:ARG:NH1	2.38	0.56
1:B:115:HIS:NE2	1:B:185:GLU:OE2	2.38	0.56
3:B:902:AGS:S1G	1:C:766:ARG:NH1	2.79	0.55
1:D:433:GLU:HG2	1:D:438:ASP:OD2	2.06	0.55
1:A:115:HIS:CD2	2:U:227:ALA:O	2.60	0.55
2:U:226:ARG:HG3	2:U:227:ALA:N	2.22	0.55
1:E:695:CYS:SG	1:F:508:MET:SD	3.04	0.55
1:F:247:PRO:HB3	3:F:901:AGS:S1G	2.47	0.54
1:F:127:THR:HG22	1:F:437:ILE:HB	1.89	0.54
1:B:635:ARG:NH1	1:B:636:PRO:O	2.39	0.54
1:F:707:ILE:HG22	1:F:708:ARG:N	2.22	0.54
1:D:434:ASP:O	1:D:435:GLU:C	2.46	0.54
1:E:203:TYR:CE2	1:E:261:GLU:HG2	2.43	0.54
1:E:542:ILE:HD13	1:E:562:ILE:HD13	1.90	0.54
3:E:902:AGS:S1G	1:F:766:ARG:NH1	2.81	0.54
1:C:420:LEU:CD1	1:D:235:VAL:HG11	2.38	0.54
2:U:230:GLY:O	2:U:231:SER:HB3	2.08	0.54
3:C:902:AGS:O2A	7:C:1001:HOH:O	2.18	0.54
1:D:696:LYS:HE2	1:E:492:LEU:HD23	1.90	0.54
2:V:230:GLY:O	2:V:231:SER:HB3	2.08	0.54
1:C:707:ILE:HG22	1:C:708:ARG:N	2.23	0.54
1:C:158:MET:N	1:C:387:ASN:O	2.40	0.54
1:D:254:ILE:HD12	1:D:369:ILE:HD13	1.90	0.53
1:B:124:GLU:OE1	1:B:125:GLY:N	2.41	0.53
1:C:237:PRO:HG2	1:C:340:HIS:HE1	1.72	0.53
1:F:136:LYS:HB3	1:F:137:PRO:HD3	1.90	0.53
1:A:650:GLU:OE1	1:A:677:LYS:HG3	2.08	0.53
1:C:615:LYS:HA	1:C:615:LYS:HE2	1.91	0.53
1:D:124:GLU:OE1	1:D:125:GLY:N	2.41	0.53
1:D:158:MET:CE	1:E:235:VAL:HG21	2.39	0.53
3:C:903:AGS:S1G	1:D:766:ARG:NH1	2.82	0.53
1:A:434:ASP:OD2	1:B:226:HIS:CE1	2.62	0.53
1:C:136:LYS:HB3	1:C:137:PRO:HD3	1.89	0.53
1:A:312:LYS:HE3	1:A:351:ASN:O	2.07	0.53
1:E:435:GLU:HG3	1:E:436:THR:N	2.24	0.53
1:B:160:ALA:HB2	1:B:387:ASN:OD1	2.09	0.53
1:A:635:ARG:NH1	1:A:636:PRO:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ARG:NH2	1:D:607:GLU:OE1	2.42	0.53
1:B:136:LYS:HB3	1:B:137:PRO:HD3	1.90	0.53
1:A:442:MET:SD	1:B:233:ILE:HD13	2.49	0.52
1:A:542:ILE:HD13	1:A:562:ILE:HD13	1.92	0.52
1:D:136:LYS:HB3	1:D:137:PRO:HD3	1.92	0.52
1:F:461:PRO:HG2	1:F:464:LEU:HD21	1.90	0.52
1:E:121:ASP:OD2	1:E:191:ARG:HD2	2.09	0.52
1:D:220:VAL:CG1	1:D:224:LEU:HD12	2.39	0.52
1:B:355:PRO:O	1:B:359:ARG:NH1	2.42	0.52
1:E:136:LYS:HB3	1:E:137:PRO:HD3	1.90	0.52
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.44	0.52
1:D:317:HIS:CE1	1:E:322:ARG:NH1	2.78	0.52
1:F:124:GLU:C	1:F:124:GLU:OE1	2.48	0.52
1:C:53:ARG:HB2	1:C:72:LEU:HD23	1.92	0.52
1:D:698:ALA:HA	1:D:735:HIS:CE1	2.44	0.52
1:C:349:ARG:HG3	1:C:352:SER:CB	2.40	0.52
1:B:430:ILE:O	1:B:431:ASP:CB	2.58	0.51
1:B:203:TYR:CE2	1:B:261:GLU:HG2	2.45	0.51
1:E:222:LEU:HB2	1:E:223:PRO:HD3	1.92	0.51
1:A:120:ASP:N	1:A:188:PRO:HB2	2.26	0.51
1:A:111:GLY:O	1:A:180:THR:HG22	2.09	0.51
1:A:313:ARG:O	1:A:316:THR:OG1	2.29	0.51
1:A:434:ASP:O	1:A:436:THR:N	2.44	0.51
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.92	0.51
1:B:430:ILE:O	1:B:431:ASP:HB2	2.10	0.51
1:C:438:ASP:OD1	1:C:440:GLU:N	2.43	0.51
1:E:105:CYS:HB3	1:E:108:VAL:HG13	1.92	0.51
1:E:339:ALA:O	1:E:340:HIS:C	2.49	0.51
1:A:431:ASP:O	1:A:433:GLU:N	2.44	0.51
1:A:508:MET:SD	1:F:695:CYS:SG	3.07	0.51
1:C:338:ARG:HG2	1:C:338:ARG:O	2.11	0.51
1:A:495:TYR:N	1:A:496:PRO:HD2	2.26	0.51
1:D:433:GLU:O	1:D:433:GLU:HG3	2.11	0.51
1:D:115:HIS:NE2	2:V:227:ALA:O	2.44	0.50
1:F:222:LEU:HB3	1:F:223:PRO:HD3	1.93	0.50
1:C:124:GLU:OE1	1:C:125:GLY:N	2.45	0.50
1:B:222:LEU:HB3	1:B:223:PRO:HD3	1.93	0.50
1:C:237:PRO:HG2	1:C:340:HIS:CE1	2.46	0.50
1:C:437:ILE:HD11	1:D:229:LEU:CD1	2.41	0.50
1:B:283:GLU:OE2	1:B:323:ARG:HD2	2.12	0.50
1:D:201:VAL:HG11	1:D:253:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ARG:C	1:C:340:HIS:N	2.63	0.50
1:C:167:GLU:HG3	1:C:168:THR:N	2.26	0.50
1:D:527:LEU:HD12	1:D:645:ILE:HD13	1.92	0.50
1:D:436:THR:OG1	1:D:437:ILE:N	2.45	0.50
1:F:94:VAL:HG12	1:F:95:ARG:N	2.26	0.50
2:V:226:ARG:CG	2:V:227:ALA:N	2.74	0.50
1:E:461:PRO:HG2	1:E:464:LEU:HD21	1.93	0.50
1:C:707:ILE:CG2	1:C:708:ARG:N	2.75	0.50
1:F:527:LEU:HD12	1:F:645:ILE:HD13	1.93	0.50
1:C:222:LEU:HB3	1:C:223:PRO:HD3	1.94	0.50
1:B:700:ARG:HG3	1:B:701:GLU:N	2.25	0.50
1:C:94:VAL:HG12	1:C:95:ARG:N	2.27	0.50
1:A:131:PHE:HD1	1:A:135:LEU:HD12	1.77	0.50
1:F:431:ASP:O	1:F:433:GLU:N	2.45	0.50
1:A:702:SER:O	1:A:706:GLU:HA	2.12	0.49
1:B:420:LEU:CD1	1:C:235:VAL:HG11	2.42	0.49
1:C:705:SER:HB2	1:C:707:ILE:CD1	2.42	0.49
1:D:124:GLU:OE1	1:D:124:GLU:C	2.50	0.49
1:F:516:PHE:CD1	1:F:645:ILE:HD11	2.46	0.49
1:B:313:ARG:O	1:B:316:THR:OG1	2.29	0.49
1:C:237:PRO:CG	1:C:340:HIS:CE1	2.95	0.49
1:D:495:TYR:N	1:D:496:PRO:HD2	2.27	0.49
1:C:527:LEU:HD12	1:C:645:ILE:HD13	1.95	0.49
1:C:762:LEU:O	1:C:765:SER:OG	2.29	0.49
1:A:152:PHE:CZ	1:A:163:PHE:HB2	2.47	0.49
1:B:542:ILE:HD13	1:B:562:ILE:HD13	1.92	0.49
1:F:158:MET:N	1:F:387:ASN:O	2.45	0.49
1:F:705:SER:HB2	1:F:707:ILE:CD1	2.43	0.49
1:C:136:LYS:HB3	1:C:137:PRO:CD	2.42	0.49
1:C:254:ILE:HD12	1:C:369:ILE:HD13	1.94	0.49
1:A:94:VAL:HG12	1:A:95:ARG:N	2.28	0.49
1:F:58:LEU:HB2	1:F:105:CYS:SG	2.53	0.49
1:D:94:VAL:HG12	1:D:95:ARG:N	2.27	0.49
1:E:707:ILE:CG2	1:E:708:ARG:N	2.74	0.49
1:E:94:VAL:HG12	1:E:95:ARG:N	2.28	0.49
1:E:450:ASP:OD1	1:E:453:ARG:NH1	2.45	0.49
1:A:359:ARG:HG2	3:F:901:AGS:S1G	2.53	0.49
1:D:339:ALA:O	1:D:340:HIS:C	2.51	0.49
1:D:317:HIS:N	1:D:317:HIS:ND1	2.61	0.49
1:F:438:ASP:OD2	1:F:441:VAL:HB	2.13	0.49
2:V:228:PHE:CD1	2:V:228:PHE:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:635:ARG:NH1	1:E:636:PRO:O	2.46	0.48
1:E:254:ILE:HD12	1:E:369:ILE:HD13	1.95	0.48
1:C:349:ARG:HG3	1:C:352:SER:HB3	1.94	0.48
1:B:427:MET:SD	1:B:432:LEU:HD21	2.53	0.48
1:F:635:ARG:NH1	1:F:636:PRO:O	2.46	0.48
1:D:96:LEU:O	1:D:225:ARG:NH2	2.47	0.48
1:D:699:ILE:HG12	1:E:506:PHE:CE2	2.49	0.48
1:A:220:VAL:CG1	1:A:224:LEU:HD12	2.43	0.48
1:F:239:ARG:HB2	1:F:335:LEU:HD12	1.94	0.48
1:B:136:LYS:HB3	1:B:137:PRO:CD	2.43	0.48
1:E:532:ALA:HB2	1:E:573:VAL:HG11	1.94	0.48
1:A:339:ALA:O	1:A:340:HIS:C	2.52	0.48
3:E:901:AGS:S1G	1:F:359:ARG:HG2	2.53	0.48
1:F:707:ILE:CG2	1:F:708:ARG:N	2.77	0.48
1:B:420:LEU:HD13	1:C:235:VAL:HG11	1.95	0.48
1:B:227:PRO:HB2	1:B:340:HIS:CE1	2.48	0.48
1:B:495:TYR:N	1:B:496:PRO:HD2	2.28	0.48
2:U:227:ALA:HB1	2:U:228:PHE:HD1	1.73	0.48
1:E:142:ALA:HB1	1:E:144:ARG:HG3	1.95	0.48
1:D:624:ASN:C	1:D:625:ARG:HG2	2.34	0.48
1:F:673:GLU:OE1	1:F:673:GLU:N	2.45	0.48
1:F:124:GLU:OE1	1:F:125:GLY:N	2.47	0.48
1:B:124:GLU:C	1:B:124:GLU:OE1	2.52	0.48
1:D:669:ASP:HB2	1:D:733:ARG:HD2	1.95	0.48
1:B:430:ILE:HG23	1:B:431:ASP:N	2.29	0.47
1:A:678:MET:HE2	1:A:678:MET:HA	1.95	0.47
1:A:316:THR:O	1:A:317:HIS:C	2.52	0.47
1:D:94:VAL:HG13	1:D:98:ASP:HB2	1.97	0.47
1:B:94:VAL:HG12	1:B:95:ARG:N	2.29	0.47
1:A:465:ARG:NH2	1:B:607:GLU:OE1	2.47	0.47
1:A:514:VAL:HG23	1:A:618:PHE:CE2	2.50	0.47
1:D:350:PRO:O	1:D:358:ARG:NH2	2.47	0.47
1:D:111:GLY:O	1:D:180:THR:HG22	2.15	0.47
1:F:136:LYS:HB3	1:F:137:PRO:CD	2.44	0.47
1:E:495:TYR:N	1:E:496:PRO:HD2	2.29	0.47
1:E:230:PHE:CZ	1:E:237:PRO:HB3	2.50	0.47
1:C:442:MET:CE	1:C:442:MET:HA	2.44	0.47
1:C:495:TYR:N	1:C:496:PRO:HD2	2.30	0.47
1:A:434:ASP:O	1:A:435:GLU:C	2.53	0.47
1:D:136:LYS:HB3	1:D:137:PRO:CD	2.45	0.47
1:F:650:GLU:OE1	1:F:677:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:HG11	1:A:253:LEU:HD12	1.96	0.47
1:B:762:LEU:O	1:B:765:SER:OG	2.31	0.47
1:C:407:VAL:CG1	1:C:408:GLY:N	2.78	0.47
1:E:355:PRO:O	1:E:359:ARG:NH1	2.48	0.47
1:D:117:LEU:HD11	2:V:225:PHE:CZ	2.50	0.47
1:E:167:GLU:HG3	1:E:168:THR:N	2.30	0.47
1:F:495:TYR:N	1:F:496:PRO:HD2	2.30	0.47
1:A:431:ASP:C	1:A:433:GLU:N	2.69	0.46
1:E:649:ASP:OD1	1:E:652:SER:OG	2.25	0.46
1:E:745:ARG:NH2	1:E:749:ASP:OD1	2.47	0.46
2:U:228:PHE:CD1	2:U:228:PHE:N	2.83	0.46
1:E:136:LYS:HB3	1:E:137:PRO:CD	2.45	0.46
1:F:431:ASP:C	1:F:433:GLU:N	2.66	0.46
1:B:416:SER:OG	1:C:235:VAL:HG13	2.16	0.46
1:B:254:ILE:HD12	1:B:369:ILE:HD13	1.98	0.46
1:F:90:ASN:O	1:F:93:ARG:NH1	2.48	0.46
1:D:573:VAL:HG23	1:D:620:ILE:CD1	2.45	0.46
1:A:527:LEU:HD12	1:A:645:ILE:HD13	1.98	0.46
1:F:53:ARG:HB2	1:F:72:LEU:HD23	1.98	0.46
1:E:316:THR:O	1:E:316:THR:HG22	2.15	0.46
1:C:248:GLY:O	1:C:407:VAL:CG1	2.64	0.46
1:F:51:LEU:HD21	1:F:104:PRO:HB3	1.98	0.46
1:A:432:LEU:O	1:A:433:GLU:HG3	2.16	0.46
1:E:762:LEU:O	1:E:765:SER:OG	2.33	0.46
1:C:532:ALA:HB2	1:C:573:VAL:HG11	1.98	0.46
1:A:63:LYS:HE2	1:A:194:GLU:OE1	2.15	0.46
1:C:635:ARG:NH1	1:C:636:PRO:O	2.49	0.46
1:F:110:TYR:N	1:F:110:TYR:CD1	2.84	0.46
1:A:232:ALA:CB	1:F:437:ILE:HD11	2.46	0.46
1:A:624:ASN:C	1:A:625:ARG:HG2	2.35	0.46
1:A:53:ARG:HB2	1:A:72:LEU:HD23	1.97	0.46
2:V:234:ARG:O	2:V:235:LEU:HB2	2.16	0.46
1:A:136:LYS:HB3	1:A:137:PRO:CD	2.46	0.46
1:B:734:ASP:OD1	1:B:735:HIS:N	2.49	0.46
1:B:524:LYS:HG2	1:B:645:ILE:HD12	1.97	0.46
1:D:414:LEU:C	1:D:414:LEU:HD12	2.36	0.46
1:D:115:HIS:CE1	2:V:227:ALA:O	2.69	0.45
1:C:111:GLY:HA2	1:C:170:PRO:HG2	1.98	0.45
1:A:126:ILE:HD12	1:A:127:THR:H	1.81	0.45
1:F:395:ASP:OD2	1:F:398:GLN:NE2	2.49	0.45
1:C:432:LEU:C	1:C:434:ASP:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:PRO:HB2	1:F:340:HIS:CE1	2.51	0.45
1:D:441:VAL:O	1:D:444:SER:OG	2.28	0.45
1:A:493:VAL:HG22	1:A:618:PHE:CD2	2.52	0.45
1:E:407:VAL:CG1	1:E:408:GLY:N	2.79	0.45
1:B:672:LEU:N	1:B:672:LEU:HD12	2.31	0.45
1:A:317:HIS:HB3	1:F:317:HIS:NE2	2.31	0.45
1:C:124:GLU:OE1	1:C:124:GLU:C	2.54	0.45
1:F:110:TYR:N	1:F:110:TYR:HD1	2.14	0.45
1:C:552:PHE:CD1	1:C:596:ALA:HB2	2.52	0.45
1:C:118:PRO:HG2	1:C:188:PRO:HB3	1.98	0.45
1:E:527:LEU:HD12	1:E:645:ILE:HD13	1.98	0.45
2:U:226:ARG:CG	2:U:227:ALA:N	2.79	0.45
1:E:230:PHE:HA	1:E:233:ILE:HG22	1.98	0.45
1:D:542:ILE:CD1	1:D:562:ILE:HD13	2.46	0.45
1:A:542:ILE:HD12	1:A:562:ILE:HG21	1.97	0.45
1:F:254:ILE:HD12	1:F:369:ILE:HD13	1.99	0.45
1:B:192:GLU:HB2	1:B:195:GLU:CD	2.37	0.45
1:F:407:VAL:CG1	1:F:408:GLY:N	2.80	0.45
1:A:762:LEU:O	1:A:765:SER:OG	2.32	0.45
1:A:672:LEU:N	1:A:672:LEU:HD12	2.31	0.45
1:C:432:LEU:O	1:C:434:ASP:N	2.49	0.45
1:C:96:LEU:CD2	1:C:96:LEU:N	2.79	0.45
1:E:551:TRP:CZ2	1:F:556:GLU:HG2	2.51	0.45
1:A:90:ASN:O	1:A:93:ARG:NH1	2.46	0.45
1:E:313:ARG:HD2	1:E:354:ASP:OD2	2.17	0.45
1:F:118:PRO:HB2	1:F:123:VAL:HG11	1.98	0.45
1:B:114:ILE:CD1	1:B:176:VAL:HG22	2.47	0.45
1:E:332:MET:O	1:E:335:LEU:HB2	2.16	0.45
1:E:240:GLY:HA3	1:E:363:PHE:HA	1.99	0.45
1:C:226:HIS:HB3	1:C:229:LEU:HD23	1.98	0.45
1:F:424:ARG:O	1:F:427:MET:HG2	2.17	0.45
1:C:437:ILE:HD11	1:D:229:LEU:HD11	1.98	0.45
1:F:108:VAL:CG1	1:F:175:ILE:HG13	2.47	0.45
1:A:669:ASP:OD1	1:A:733:ARG:HB2	2.16	0.45
1:F:220:VAL:CG1	1:F:224:LEU:HD12	2.47	0.45
1:E:731:ILE:HG13	1:E:731:ILE:O	2.17	0.45
2:V:227:ALA:HB1	2:V:228:PHE:HD1	1.69	0.44
1:D:311:PRO:HG2	1:D:316:THR:HG22	2.00	0.44
1:B:407:VAL:CG1	1:B:408:GLY:N	2.80	0.44
1:E:434:ASP:N	1:E:434:ASP:OD1	2.50	0.44
1:A:134:TYR:CD2	1:A:161:VAL:HG11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:234:ARG:O	2:U:235:LEU:HB2	2.17	0.44
1:A:51:LEU:HD21	1:A:104:PRO:HB3	1.98	0.44
1:C:127:THR:O	1:C:438:ASP:HA	2.18	0.44
1:A:94:VAL:HG13	1:A:98:ASP:CB	2.47	0.44
1:A:85:ASN:OD1	1:A:86:ARG:N	2.51	0.44
1:A:532:ALA:HB2	1:A:573:VAL:HG11	1.99	0.44
1:B:423:ILE:O	1:B:427:MET:N	2.51	0.44
1:C:89:ARG:NH1	1:C:96:LEU:HD21	2.33	0.44
1:D:547:LEU:HD12	1:D:582:ILE:HD11	2.00	0.44
1:E:672:LEU:N	1:E:672:LEU:HD12	2.33	0.44
1:D:420:LEU:HD21	1:E:230:PHE:CZ	2.52	0.44
1:A:461:PRO:HG2	1:A:464:LEU:HD11	1.99	0.44
1:C:686:ASP:OD1	1:C:746:SER:OG	2.29	0.44
1:C:698:ALA:HA	1:C:735:HIS:CE1	2.53	0.44
1:C:259:ALA:HB2	1:C:266:PHE:CD1	2.52	0.44
1:D:312:LYS:N	1:D:352:SER:O	2.49	0.44
1:B:201:VAL:HG11	1:B:253:LEU:HD12	2.00	0.44
1:D:131:PHE:CZ	2:V:234:ARG:NH1	2.85	0.43
1:A:94:VAL:CG1	1:A:98:ASP:HB2	2.48	0.43
1:A:707:ILE:HG23	1:A:708:ARG:N	2.32	0.43
1:C:624:ASN:C	1:C:625:ARG:HG2	2.38	0.43
1:E:141:GLU:O	1:E:141:GLU:CD	2.57	0.43
1:E:624:ASN:C	1:E:625:ARG:HG2	2.37	0.43
1:A:423:ILE:O	1:A:427:MET:HB2	2.18	0.43
1:A:134:TYR:CE2	1:A:161:VAL:HG11	2.54	0.43
1:C:501:ASP:OD1	1:C:502:LYS:N	2.51	0.43
1:E:734:ASP:OD1	1:E:734:ASP:N	2.49	0.43
2:V:225:PHE:CG	2:V:226:ARG:N	2.86	0.43
1:E:320:VAL:HB	1:F:319:GLU:OE1	2.18	0.43
1:D:89:ARG:NH1	1:D:96:LEU:HD21	2.33	0.43
1:D:627:ASP:HB3	1:D:758:PHE:CZ	2.53	0.43
1:A:403:THR:HB	1:A:406:HIS:CG	2.54	0.43
1:B:501:ASP:OD1	1:B:502:LYS:N	2.51	0.43
1:A:243:LEU:O	1:A:346:ALA:HA	2.19	0.43
1:E:519:PRO:HA	1:E:755:TYR:CE2	2.54	0.43
1:A:407:VAL:CG1	1:A:408:GLY:N	2.81	0.43
1:B:682:PHE:CD1	1:B:745:ARG:HG3	2.53	0.43
1:F:167:GLU:HG3	1:F:168:THR:N	2.32	0.43
1:A:158:MET:HE3	1:B:235:VAL:HG21	2.00	0.43
1:C:625:ARG:HD2	1:D:767:GLY:O	2.18	0.43
1:B:332:MET:O	1:B:335:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:LYS:NZ	3:E:901:AGS:O1B	2.51	0.43
1:E:542:ILE:HD12	1:E:562:ILE:HG21	1.99	0.43
1:A:120:ASP:CA	1:A:188:PRO:HB2	2.48	0.43
1:D:729:PRO:HB2	1:E:506:PHE:CZ	2.54	0.43
1:E:122:THR:HB	1:E:161:VAL:HA	2.01	0.43
1:B:627:ASP:HB3	1:B:758:PHE:CZ	2.54	0.43
1:B:197:SER:HB3	1:B:200:GLU:HG2	2.01	0.43
1:A:147:ARG:NH1	1:A:172:PRO:HB2	2.33	0.43
1:B:220:VAL:CG1	1:B:224:LEU:HD22	2.49	0.43
1:F:501:ASP:OD1	1:F:502:LYS:N	2.51	0.43
1:A:312:LYS:N	1:A:352:SER:O	2.52	0.43
1:E:524:LYS:HG2	1:E:645:ILE:HD12	2.01	0.43
1:F:552:PHE:CD1	1:F:596:ALA:HB2	2.53	0.43
1:B:532:ALA:HB2	1:B:573:VAL:HG11	1.99	0.43
1:A:491:GLU:OE2	1:F:700:ARG:NE	2.51	0.43
1:B:624:ASN:C	1:B:625:ARG:HG2	2.38	0.43
1:D:461:PRO:O	1:D:464:LEU:HD11	2.18	0.43
1:A:317:HIS:CE1	1:B:322:ARG:NH1	2.87	0.42
1:E:191:ARG:NH1	1:E:191:ARG:HB3	2.34	0.42
1:C:89:ARG:HD3	1:C:96:LEU:HD22	2.01	0.42
1:A:556:GLU:HA	1:A:603:GLN:OE1	2.19	0.42
1:C:58:LEU:HB2	1:C:105:CYS:SG	2.58	0.42
1:F:313:ARG:O	1:F:316:THR:OG1	2.32	0.42
1:A:380:ILE:CD1	3:A:901:AGS:N1	2.82	0.42
1:C:118:PRO:HG3	1:C:130:LEU:HD13	2.01	0.42
1:F:313:ARG:NE	1:F:354:ASP:OD2	2.53	0.42
1:A:515:LEU:HD22	1:A:634:LEU:HD21	2.00	0.42
1:A:58:LEU:HB2	1:A:105:CYS:SG	2.58	0.42
1:A:627:ASP:HB3	1:A:758:PHE:CZ	2.54	0.42
1:D:433:GLU:O	1:D:434:ASP:C	2.57	0.42
1:E:698:ALA:CB	1:E:731:ILE:HG22	2.50	0.42
1:F:230:PHE:CE1	1:F:237:PRO:HB3	2.54	0.42
1:A:675:LEU:HD11	1:A:740:MET:HE3	2.02	0.42
1:F:406:HIS:CE1	1:F:461:PRO:HB3	2.54	0.42
1:B:425:LYS:HG3	1:B:426:LYS:N	2.33	0.42
1:B:243:LEU:O	1:B:346:ALA:HA	2.19	0.42
1:E:350:PRO:O	1:E:358:ARG:NH2	2.53	0.42
1:F:125:GLY:O	1:F:437:ILE:HG13	2.20	0.42
1:D:438:ASP:HB3	1:D:441:VAL:HB	2.01	0.42
1:B:527:LEU:HD12	1:B:645:ILE:HD13	2.02	0.42
1:B:376:GLY:O	1:B:379:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:225:PHE:CD1	2:V:225:PHE:C	2.93	0.42
1:D:532:ALA:HB2	1:D:573:VAL:HG11	2.00	0.42
1:D:120:ASP:N	1:D:188:PRO:HB2	2.35	0.42
1:D:407:VAL:CG1	1:D:408:GLY:N	2.81	0.42
1:D:115:HIS:CD2	2:V:227:ALA:O	2.73	0.42
1:A:442:MET:SD	1:B:233:ILE:CD1	3.07	0.42
1:C:349:ARG:HA	1:C:350:PRO:HD2	1.90	0.42
1:A:131:PHE:HE1	1:A:182:ILE:HD13	1.83	0.42
1:F:159:ARG:N	1:F:387:ASN:HB3	2.35	0.42
1:A:94:VAL:HG13	1:A:98:ASP:HB2	2.02	0.42
1:E:230:PHE:CE1	1:E:237:PRO:HB3	2.55	0.42
1:A:501:ASP:OD1	1:A:502:LYS:N	2.52	0.42
1:D:349:ARG:HA	1:D:350:PRO:HD2	1.92	0.42
1:D:542:ILE:HD13	1:D:562:ILE:HD13	1.99	0.42
1:A:167:GLU:HG3	1:A:168:THR:N	2.33	0.42
1:A:442:MET:HA	1:A:442:MET:CE	2.49	0.42
1:F:321:GLU:HA	1:F:324:ILE:HD12	2.01	0.42
1:E:127:THR:O	1:E:438:ASP:HA	2.19	0.42
1:E:22:ARG:HB2	1:E:22:ARG:NH1	2.35	0.42
1:E:269:ILE:HD11	1:E:289:ALA:CB	2.50	0.42
1:E:141:GLU:CG	1:E:141:GLU:O	2.67	0.42
1:B:573:VAL:CG2	1:B:620:ILE:HD12	2.50	0.42
1:E:317:HIS:O	1:F:322:ARG:NH2	2.53	0.42
1:E:43:GLN:N	1:E:44:PRO:CD	2.83	0.41
1:E:203:TYR:CE2	1:E:217:LYS:HD3	2.54	0.41
1:A:28:VAL:HG21	1:A:94:VAL:HG11	2.02	0.41
1:B:248:GLY:O	1:B:407:VAL:CG1	2.68	0.41
1:D:514:VAL:HG12	1:D:515:LEU:N	2.34	0.41
1:E:501:ASP:OD1	1:E:502:LYS:N	2.52	0.41
1:E:231:LYS:C	1:E:231:LYS:HD3	2.40	0.41
1:F:532:ALA:HB2	1:F:573:VAL:HG11	2.01	0.41
1:A:559:VAL:HA	1:A:562:ILE:HD12	2.02	0.41
1:F:126:ILE:HD11	1:F:159:ARG:HD3	2.02	0.41
1:D:635:ARG:NH1	1:D:636:PRO:O	2.53	0.41
1:C:277:LYS:HB3	1:C:281:GLU:HB3	2.02	0.41
1:B:427:MET:O	1:B:429:LEU:N	2.53	0.41
1:A:143:TYR:CE2	1:A:178:PRO:HD3	2.54	0.41
1:B:115:HIS:NE2	1:B:185:GLU:HG3	2.35	0.41
1:C:732:ARG:NH1	1:C:735:HIS:CE1	2.88	0.41
1:F:22:ARG:HG2	1:F:23:PRO:HD2	2.02	0.41
1:F:111:GLY:HA2	1:F:170:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ILE:HD13	1:C:99:VAL:HG13	2.01	0.41
1:A:732:ARG:NE	1:A:734:ASP:OD2	2.53	0.41
1:D:501:ASP:OD1	1:D:502:LYS:N	2.53	0.41
1:A:115:HIS:CE1	2:U:227:ALA:O	2.74	0.41
1:D:94:VAL:CG1	1:D:98:ASP:HB2	2.51	0.41
1:E:313:ARG:CD	1:E:354:ASP:OD2	2.68	0.41
1:F:482:LEU:O	1:F:486:LYS:HG3	2.21	0.41
1:D:321:GLU:OE2	1:E:322:ARG:HD2	2.20	0.41
1:E:573:VAL:HG23	1:E:620:ILE:HD12	2.03	0.41
1:E:476:TRP:CE3	1:E:486:LYS:HD3	2.55	0.41
1:B:731:ILE:HD11	1:B:736:PHE:CE2	2.55	0.41
1:F:672:LEU:HD12	1:F:672:LEU:N	2.36	0.41
1:A:734:ASP:OD1	1:A:734:ASP:N	2.36	0.41
1:E:769:GLY:O	1:E:770:SER:C	2.59	0.41
1:D:430:ILE:HG22	1:D:431:ASP:N	2.35	0.41
1:A:435:GLU:HG3	1:A:436:THR:N	2.35	0.41
1:E:435:GLU:CG	1:E:436:THR:N	2.84	0.41
1:B:142:ALA:O	1:B:143:TYR:CG	2.74	0.41
1:B:230:PHE:CE1	1:B:237:PRO:HB3	2.56	0.41
1:D:94:VAL:HG13	1:D:98:ASP:CB	2.50	0.41
1:F:627:ASP:HB3	1:F:758:PHE:CZ	2.55	0.41
1:B:423:ILE:O	1:B:427:MET:HB2	2.21	0.41
1:B:113:ARG:HG2	1:B:169:ASP:HB2	2.03	0.41
1:D:98:ASP:OD1	1:D:225:ARG:NH1	2.51	0.41
1:B:434:ASP:O	1:B:435:GLU:C	2.57	0.41
1:B:478:ASP:OD1	1:B:662:ARG:NH2	2.53	0.41
1:D:461:PRO:HG2	1:D:464:LEU:HD11	2.02	0.41
1:D:120:ASP:CA	1:D:188:PRO:HB2	2.51	0.41
1:D:222:LEU:HB2	1:D:223:PRO:CD	2.51	0.40
1:B:705:SER:OG	1:B:706:GLU:N	2.50	0.40
1:E:224:LEU:HD21	1:E:300:ILE:HG13	2.03	0.40
1:E:514:VAL:HG12	1:E:515:LEU:N	2.36	0.40
1:A:429:LEU:HD12	1:A:429:LEU:H	1.86	0.40
1:F:428:ASP:O	1:F:431:ASP:HB3	2.21	0.40
1:D:658:LYS:O	1:D:662:ARG:HG3	2.21	0.40
1:D:762:LEU:O	1:D:765:SER:OG	2.38	0.40
1:E:442:MET:CE	1:F:233:ILE:HD13	2.50	0.40
1:A:307:ASP:N	1:A:307:ASP:OD1	2.55	0.40
1:F:514:VAL:HG12	1:F:515:LEU:N	2.36	0.40
1:D:706:GLU:CA	1:D:706:GLU:OE2	2.69	0.40
1:B:85:ASN:OD1	1:B:86:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:LEU:HD21	1:C:740:MET:CE	2.52	0.40
1:E:427:MET:SD	1:E:445:LEU:HD12	2.62	0.40
1:C:159:ARG:N	1:C:387:ASN:HB3	2.36	0.40
1:A:134:TYR:CE2	1:A:161:VAL:CG1	3.04	0.40
1:D:115:HIS:ND1	1:D:183:HIS:O	2.55	0.40
1:A:231:LYS:HD3	1:A:231:LYS:C	2.42	0.40
1:B:437:ILE:HG12	1:C:229:LEU:HD12	2.04	0.40
1:E:519:PRO:HA	1:E:520:PRO:HD3	1.95	0.40
1:A:27:ILE:HB	1:A:81:LYS:HG2	2.04	0.40
1:B:146:ILE:HD11	1:B:168:THR:HG21	2.04	0.40
1:C:519:PRO:HA	1:C:520:PRO:HD3	1.94	0.40
1:C:535:CYS:O	1:C:536:GLN:CG	2.70	0.40
1:D:164:LYS:HE2	1:D:189:ILE:HD13	2.04	0.40

All (2) 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)
1:C:284:SER:OG	1:F:671:ASP:OD2[3_555]	2.02	0.18
1:A:112:LYS:NZ	1:D:397:GLU:OE1[1_455]	2.17	0.03

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	720/785 (92%)	690 (96%)	25 (4%)	5 (1%)	26	65
1	B	720/785 (92%)	696 (97%)	20 (3%)	4 (1%)	30	68
1	C	720/785 (92%)	698 (97%)	20 (3%)	2 (0%)	46	80
1	D	720/785 (92%)	697 (97%)	21 (3%)	2 (0%)	46	80
1	E	720/785 (92%)	695 (96%)	20 (3%)	5 (1%)	26	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	720/785 (92%)	693 (96%)	23 (3%)	4 (1%)	30	68
2	U	8/21 (38%)	1 (12%)	3 (38%)	4 (50%)	0	0
2	V	9/21 (43%)	2 (22%)	3 (33%)	4 (44%)	0	0
All	All	4337/4752 (91%)	4172 (96%)	135 (3%)	30 (1%)	26	65

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	HIS
1	B	428	ASP
1	B	430	ILE
1	B	431	ASP
1	C	706	GLU
1	D	340	HIS
1	E	340	HIS
1	F	340	HIS
2	V	229	SER
2	V	233	ASN
2	U	229	SER
2	U	233	ASN
1	A	432	LEU
1	A	435	GLU
1	B	340	HIS
1	E	435	GLU
1	E	706	GLU
1	F	432	LEU
1	E	431	ASP
1	A	706	GLU
1	C	433	GLU
1	D	339	ALA
2	V	227	ALA
2	V	231	SER
2	U	227	ALA
2	U	231	SER
1	A	434	ASP
1	E	339	ALA
1	F	433	GLU
1	F	706	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	617/658 (94%)	561 (91%)	56 (9%)	12	40
1	B	617/658 (94%)	583 (94%)	34 (6%)	27	63
1	C	617/658 (94%)	563 (91%)	54 (9%)	12	44
1	D	617/658 (94%)	573 (93%)	44 (7%)	18	54
1	E	617/658 (94%)	576 (93%)	41 (7%)	21	56
1	F	617/658 (94%)	584 (95%)	33 (5%)	28	64
2	U	7/14 (50%)	6 (86%)	1 (14%)	4	17
2	V	8/14 (57%)	6 (75%)	2 (25%)	1	2
All	All	3717/3976 (94%)	3452 (93%)	265 (7%)	18	54

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	45	LYS
1	A	52	PHE
1	A	78	SER
1	A	79	ASP
1	A	90	ASN
1	A	99	VAL
1	A	105	CYS
1	A	126	ILE
1	A	147	ARG
1	A	155	ARG
1	A	159	ARG
1	A	171	SER
1	A	181	VAL
1	A	190	LYS
1	A	229	LEU
1	A	230	PHE
1	A	231	LYS
1	A	236	LYS

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Mol	Chain	Res	Type
1	A	274	ILE
1	A	295	LYS
1	A	313	ARG
1	A	317	HIS
1	A	335	LEU
1	A	336	LYS
1	A	355	PRO
1	A	359	ARG
1	A	365	ARG
1	A	378	LEU
1	A	414	LEU
1	A	416	SER
1	A	425	LYS
1	A	427	MET
1	A	429	LEU
1	A	432	LEU
1	A	435	GLU
1	A	442	MET
1	A	443	ASN
1	A	458	GLN
1	A	487	ARG
1	A	509	THR
1	A	551	TRP
1	A	556	GLU
1	A	573	VAL
1	A	599	ARG
1	A	625	ARG
1	A	678	MET
1	A	700	ARG
1	A	705	SER
1	A	708	ARG
1	A	734	ASP
1	A	738	GLU
1	A	757	MET
1	A	762	LEU
1	A	765	SER
1	A	770	SER
1	B	45	LYS
1	B	49	LEU
1	B	79	ASP
1	B	99	VAL
1	B	105	CYS

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Mol	Chain	Res	Type
1	B	124	GLU
1	B	131	PHE
1	B	147	ARG
1	B	155	ARG
1	B	193	ASP
1	B	236	LYS
1	B	256	ARG
1	B	261	GLU
1	B	268	LEU
1	B	284	SER
1	B	295	LYS
1	B	317	HIS
1	B	335	LEU
1	B	349	ARG
1	B	359	ARG
1	B	402	GLU
1	B	416	SER
1	B	425	LYS
1	B	431	ASP
1	B	464	LEU
1	B	509	THR
1	B	556	GLU
1	B	573	VAL
1	B	599	ARG
1	B	625	ARG
1	B	731	ILE
1	B	762	LEU
1	B	765	SER
1	B	770	SER
1	C	21	ASN
1	C	22	ARG
1	C	25	ARG
1	C	45	LYS
1	C	52	PHE
1	C	79	ASP
1	C	96	LEU
1	C	99	VAL
1	C	105	CYS
1	C	109	LYS
1	C	124	GLU
1	C	126	ILE
1	C	131	PHE

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Mol	Chain	Res	Type
1	C	155	ARG
1	C	159	ARG
1	C	173	TYR
1	C	230	PHE
1	C	233	ILE
1	C	236	LYS
1	C	256	ARG
1	C	283	GLU
1	C	284	SER
1	C	292	GLU
1	C	295	LYS
1	C	313	ARG
1	C	336	LYS
1	C	340	HIS
1	C	355	PRO
1	C	359	ARG
1	C	365	ARG
1	C	402	GLU
1	C	416	SER
1	C	424	ARG
1	C	432	LEU
1	C	433	GLU
1	C	436	THR
1	C	437	ILE
1	C	442	MET
1	C	443	ASN
1	C	445	LEU
1	C	498	GLU
1	C	509	THR
1	C	556	GLU
1	C	573	VAL
1	C	614	LYS
1	C	615	LYS
1	C	625	ARG
1	C	675	LEU
1	C	700	ARG
1	C	705	SER
1	C	708	ARG
1	C	732	ARG
1	C	762	LEU
1	C	765	SER
1	D	22	ARG

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Mol	Chain	Res	Type
1	D	45	LYS
1	D	78	SER
1	D	79	ASP
1	D	99	VAL
1	D	105	CYS
1	D	124	GLU
1	D	131	PHE
1	D	147	ARG
1	D	155	ARG
1	D	159	ARG
1	D	167	GLU
1	D	181	VAL
1	D	189	ILE
1	D	193	ASP
1	D	230	PHE
1	D	236	LYS
1	D	283	GLU
1	D	284	SER
1	D	295	LYS
1	D	315	LYS
1	D	317	HIS
1	D	322	ARG
1	D	335	LEU
1	D	349	ARG
1	D	359	ARG
1	D	414	LEU
1	D	429	LEU
1	D	430	ILE
1	D	436	THR
1	D	443	ASN
1	D	487	ARG
1	D	509	THR
1	D	556	GLU
1	D	573	VAL
1	D	599	ARG
1	D	618	PHE
1	D	625	ARG
1	D	700	ARG
1	D	706	GLU
1	D	757	MET
1	D	762	LEU
1	D	765	SER

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Mol	Chain	Res	Type
1	D	770	SER
1	E	46	MET
1	E	49	LEU
1	E	79	ASP
1	E	90	ASN
1	E	99	VAL
1	E	105	CYS
1	E	107	ASP
1	E	113	ARG
1	E	124	GLU
1	E	131	PHE
1	E	147	ARG
1	E	155	ARG
1	E	171	SER
1	E	230	PHE
1	E	231	LYS
1	E	256	ARG
1	E	261	GLU
1	E	284	SER
1	E	295	LYS
1	E	313	ARG
1	E	335	LEU
1	E	349	ARG
1	E	359	ARG
1	E	365	ARG
1	E	416	SER
1	E	428	ASP
1	E	429	LEU
1	E	435	GLU
1	E	464	LEU
1	E	478	ASP
1	E	509	THR
1	E	556	GLU
1	E	573	VAL
1	E	599	ARG
1	E	625	ARG
1	E	700	ARG
1	E	734	ASP
1	E	757	MET
1	E	762	LEU
1	E	765	SER
1	E	768	PHE

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Mol	Chain	Res	Type
1	F	45	LYS
1	F	52	PHE
1	F	99	VAL
1	F	124	GLU
1	F	131	PHE
1	F	147	ARG
1	F	155	ARG
1	F	173	TYR
1	F	193	ASP
1	F	284	SER
1	F	287	ARG
1	F	295	LYS
1	F	313	ARG
1	F	336	LYS
1	F	338	ARG
1	F	349	ARG
1	F	359	ARG
1	F	365	ARG
1	F	401	ASN
1	F	402	GLU
1	F	431	ASP
1	F	464	LEU
1	F	487	ARG
1	F	509	THR
1	F	556	GLU
1	F	573	VAL
1	F	675	LEU
1	F	693	ARG
1	F	700	ARG
1	F	705	SER
1	F	734	ASP
1	F	738	GLU
1	F	762	LEU
2	V	225	PHE
2	V	228	PHE
2	U	228	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	340	HIS
1	D	90	ASN

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 32 ligands modelled in this entry, 18 are monoatomic - leaving 14 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	AGS	A	901	4	26,33,33	1.43	6 (23%)	24,52,52	2.57	2 (8%)
3	AGS	A	902	4	26,33,33	1.41	6 (23%)	24,52,52	2.57	3 (12%)
3	AGS	B	901	4	26,33,33	1.40	6 (23%)	24,52,52	2.62	1 (4%)
3	AGS	B	902	4	26,33,33	1.41	6 (23%)	24,52,52	2.57	4 (16%)
3	AGS	C	902	4	26,33,33	1.44	6 (23%)	24,52,52	2.49	2 (8%)
3	AGS	C	903	4	26,33,33	1.43	6 (23%)	24,52,52	2.53	2 (8%)
3	AGS	D	902	4	26,33,33	1.43	6 (23%)	24,52,52	2.53	3 (12%)
3	AGS	D	903	4	26,33,33	1.41	6 (23%)	24,52,52	2.50	2 (8%)
3	AGS	E	901	4	26,33,33	1.46	7 (26%)	24,52,52	2.61	4 (16%)
3	AGS	E	902	4	26,33,33	1.42	6 (23%)	24,52,52	2.48	2 (8%)
3	AGS	F	901	4	26,33,33	1.39	6 (23%)	24,52,52	2.56	3 (12%)
3	AGS	F	902	4	26,33,33	1.43	6 (23%)	24,52,52	2.53	3 (12%)
6	GOL	F	906	-	5,5,5	0.41	0	5,5,5	0.18	0
6	GOL	F	907	-	5,5,5	0.35	0	5,5,5	0.22	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
3	AGS	A	901	4	-	0/17/38/38	0/3/3/3
3	AGS	A	902	4	-	0/17/38/38	0/3/3/3
3	AGS	B	901	4	-	0/17/38/38	0/3/3/3
3	AGS	B	902	4	-	0/17/38/38	0/3/3/3
3	AGS	C	902	4	-	0/17/38/38	0/3/3/3
3	AGS	C	903	4	-	0/17/38/38	0/3/3/3
3	AGS	D	902	4	-	0/17/38/38	0/3/3/3
3	AGS	D	903	4	-	0/17/38/38	0/3/3/3
3	AGS	E	901	4	-	0/17/38/38	0/3/3/3
3	AGS	E	902	4	-	0/17/38/38	0/3/3/3
3	AGS	F	901	4	-	0/17/38/38	0/3/3/3
3	AGS	F	902	4	-	0/17/38/38	0/3/3/3
6	GOL	F	906	-	-	0/4/4/4	0/0/0/0
6	GOL	F	907	-	-	0/4/4/4	0/0/0/0

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	AGS	O2'-C2'	-2.55	1.37	1.43
3	B	901	AGS	O2'-C2'	-2.53	1.37	1.43
3	C	902	AGS	O2'-C2'	-2.52	1.37	1.43
3	C	903	AGS	O2'-C2'	-2.50	1.37	1.43
3	E	902	AGS	O2'-C2'	-2.48	1.37	1.43
3	E	901	AGS	C2'-C1'	-2.47	1.49	1.53
3	B	902	AGS	O2'-C2'	-2.46	1.37	1.43
3	D	903	AGS	O2'-C2'	-2.46	1.37	1.43
3	A	902	AGS	O2'-C2'	-2.45	1.37	1.43
3	D	902	AGS	O2'-C2'	-2.45	1.37	1.43
3	E	901	AGS	O2'-C2'	-2.44	1.37	1.43
3	F	901	AGS	O2'-C2'	-2.44	1.37	1.43
3	F	902	AGS	O2'-C2'	-2.43	1.37	1.43
3	A	901	AGS	C2'-C3'	-2.38	1.47	1.53
3	C	902	AGS	C2'-C3'	-2.34	1.47	1.53
3	F	902	AGS	C2'-C3'	-2.33	1.47	1.53
3	A	902	AGS	C2'-C3'	-2.30	1.47	1.53
3	C	903	AGS	C2'-C3'	-2.30	1.47	1.53
3	A	901	AGS	O3'-C3'	-2.28	1.37	1.43
3	B	902	AGS	C2'-C3'	-2.28	1.47	1.53
3	D	902	AGS	O3'-C3'	-2.27	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	AGS	C2'-C3'	-2.25	1.47	1.53
3	C	902	AGS	O3'-C3'	-2.25	1.37	1.43
3	D	902	AGS	C2'-C3'	-2.24	1.47	1.53
3	F	901	AGS	C2'-C3'	-2.21	1.47	1.53
3	D	903	AGS	C2'-C3'	-2.21	1.47	1.53
3	F	902	AGS	O3'-C3'	-2.20	1.37	1.43
3	A	902	AGS	O3'-C3'	-2.19	1.37	1.43
3	D	903	AGS	O3'-C3'	-2.19	1.37	1.43
3	E	902	AGS	O3'-C3'	-2.19	1.37	1.43
3	C	903	AGS	O3'-C3'	-2.19	1.37	1.43
3	B	902	AGS	O3'-C3'	-2.18	1.37	1.43
3	F	901	AGS	O3'-C3'	-2.18	1.37	1.43
3	E	902	AGS	C2'-C3'	-2.14	1.47	1.53
3	E	901	AGS	O3'-C3'	-2.12	1.38	1.43
3	E	901	AGS	C2'-C3'	-2.07	1.47	1.53
3	B	901	AGS	O3'-C3'	-2.07	1.38	1.43
3	A	901	AGS	PG-S1G	2.04	1.94	1.90
3	B	902	AGS	PG-S1G	2.18	1.94	1.90
3	F	901	AGS	PG-S1G	2.22	1.94	1.90
3	E	902	AGS	PG-S1G	2.26	1.94	1.90
3	A	902	AGS	PG-S1G	2.30	1.94	1.90
3	D	902	AGS	PG-S1G	2.33	1.94	1.90
3	B	901	AGS	PG-S1G	2.34	1.94	1.90
3	D	903	AGS	PG-S1G	2.36	1.94	1.90
3	C	902	AGS	PG-S1G	2.36	1.94	1.90
3	C	903	AGS	PG-S1G	2.37	1.94	1.90
3	F	902	AGS	PG-S1G	2.37	1.94	1.90
3	B	901	AGS	C2-N3	2.40	1.36	1.32
3	E	901	AGS	C6-N6	2.41	1.44	1.34
3	E	901	AGS	PG-S1G	2.42	1.95	1.90
3	F	901	AGS	C6-N6	2.48	1.44	1.34
3	A	902	AGS	C6-N6	2.49	1.44	1.34
3	C	903	AGS	C6-N6	2.50	1.44	1.34
3	D	903	AGS	C6-N6	2.50	1.44	1.34
3	C	902	AGS	C6-N6	2.51	1.44	1.34
3	A	901	AGS	C6-N6	2.51	1.44	1.34
3	B	902	AGS	C6-N6	2.51	1.44	1.34
3	F	902	AGS	C6-N6	2.51	1.44	1.34
3	D	902	AGS	C6-N6	2.52	1.44	1.34
3	E	902	AGS	C6-N6	2.53	1.44	1.34
3	B	901	AGS	C6-N6	2.57	1.44	1.34
3	F	901	AGS	C2-N3	2.72	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	AGS	C2-N3	2.73	1.37	1.32
3	A	902	AGS	C2-N3	2.79	1.37	1.32
3	F	902	AGS	C2-N3	2.79	1.37	1.32
3	B	902	AGS	C2-N3	2.79	1.37	1.32
3	D	902	AGS	C2-N3	2.79	1.37	1.32
3	C	902	AGS	C2-N3	2.83	1.37	1.32
3	E	902	AGS	C2-N3	2.85	1.37	1.32
3	C	903	AGS	C2-N3	2.86	1.37	1.32
3	D	903	AGS	C2-N3	2.87	1.37	1.32
3	E	901	AGS	C2-N3	2.96	1.37	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	AGS	N3-C2-N1	-11.71	119.67	128.87
3	A	902	AGS	N3-C2-N1	-11.55	119.80	128.87
3	B	902	AGS	N3-C2-N1	-11.36	119.95	128.87
3	C	903	AGS	N3-C2-N1	-11.31	119.98	128.87
3	F	902	AGS	N3-C2-N1	-11.31	119.99	128.87
3	F	901	AGS	N3-C2-N1	-11.31	119.99	128.87
3	D	903	AGS	N3-C2-N1	-11.24	120.04	128.87
3	D	902	AGS	N3-C2-N1	-11.23	120.05	128.87
3	A	901	AGS	N3-C2-N1	-11.23	120.05	128.87
3	E	901	AGS	N3-C2-N1	-11.22	120.06	128.87
3	E	902	AGS	N3-C2-N1	-11.17	120.10	128.87
3	C	902	AGS	N3-C2-N1	-11.15	120.11	128.87
3	A	901	AGS	PB-O3B-PG	-3.75	119.11	132.71
3	F	901	AGS	PB-O3B-PG	-3.06	121.62	132.71
3	E	901	AGS	PB-O3B-PG	-2.95	122.00	132.71
3	D	902	AGS	PB-O3B-PG	-2.73	122.80	132.71
3	B	902	AGS	PB-O3B-PG	-2.67	123.03	132.71
3	C	903	AGS	PB-O3B-PG	-2.62	123.20	132.71
3	C	902	AGS	PB-O3B-PG	-2.61	123.24	132.71
3	A	902	AGS	PB-O3B-PG	-2.57	123.37	132.71
3	E	902	AGS	PB-O3B-PG	-2.34	124.21	132.71
3	E	901	AGS	C5'-C4'-C3'	-2.29	106.33	115.20
3	F	902	AGS	PB-O3B-PG	-2.20	124.73	132.71
3	D	903	AGS	PB-O3B-PG	-2.18	124.81	132.71
3	A	902	AGS	O4'-C1'-N9	2.03	111.94	108.11
3	B	902	AGS	O4'-C4'-C3'	2.04	109.31	105.16
3	F	901	AGS	O4'-C4'-C3'	2.12	109.46	105.16
3	F	902	AGS	O4'-C1'-N9	2.17	112.21	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	AGS	O4'-C1'-N9	2.23	112.33	108.11
3	D	902	AGS	O4'-C4'-C3'	2.33	109.88	105.16
3	E	901	AGS	O4'-C1'-N9	3.30	114.34	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	AGS	4	0
3	B	902	AGS	1	0
3	C	902	AGS	2	0
3	C	903	AGS	1	0
3	D	902	AGS	1	0
3	E	901	AGS	3	0
3	E	902	AGS	1	0
3	F	901	AGS	3	0
3	F	902	AGS	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	724/785 (92%)	0.35	29 (4%)	42	20	69, 126, 205, 276	0
1	B	724/785 (92%)	0.14	18 (2%)	61	37	66, 118, 184, 264	0
1	C	724/785 (92%)	0.19	18 (2%)	61	37	55, 121, 199, 301	0
1	D	724/785 (92%)	0.24	34 (4%)	35	16	68, 130, 211, 317	0
1	E	724/785 (92%)	0.17	17 (2%)	64	40	75, 121, 192, 287	0
1	F	724/785 (92%)	0.52	70 (9%)	10	3	68, 131, 258, 320	0
2	U	10/21 (47%)	0.79	2 (20%)	1	0	170, 229, 262, 283	0
2	V	11/21 (52%)	1.05	1 (9%)	11	4	167, 186, 232, 328	0
All	All	4365/4752 (91%)	0.27	189 (4%)	39	18	55, 124, 217, 328	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	164	LYS	7.2
1	F	166	VAL	7.0
1	F	116	VAL	6.8
1	F	117	LEU	6.7
1	A	139	PHE	5.6
1	B	552	PHE	5.5
1	F	176	VAL	5.5
1	F	41	LEU	5.5
1	F	43	GLN	5.4
1	F	594	GLY	5.4
1	F	173	TYR	5.3
1	F	187	GLU	5.2
1	A	115	HIS	5.1
1	A	176	VAL	5.0
1	A	114	ILE	4.8
1	F	130	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	587	GLY	4.6
1	C	587	GLY	4.5
1	F	172	PRO	4.5
1	F	179	ASP	4.4
1	F	452	PHE	4.4
1	F	134	TYR	4.3
2	V	234	ARG	4.2
1	F	104	PRO	4.1
1	B	102	ILE	4.1
1	B	551	TRP	4.1
1	A	108	VAL	4.0
1	D	436	THR	4.0
1	A	184	CYS	3.9
1	F	102	ILE	3.8
1	A	50	GLN	3.8
1	F	508	MET	3.8
1	F	174	CYS	3.7
1	E	427	MET	3.7
1	C	23	PRO	3.6
1	F	125	GLY	3.6
1	F	139	PHE	3.6
1	D	186	GLY	3.6
1	F	190	LYS	3.6
1	F	167	GLU	3.6
1	E	668	LYS	3.6
1	F	50	GLN	3.6
1	D	708	ARG	3.5
1	F	23	PRO	3.5
1	F	235	VAL	3.5
1	A	708	ARG	3.5
1	F	426	LYS	3.4
1	B	46	MET	3.4
1	D	117	LEU	3.4
1	A	594	GLY	3.4
1	C	552	PHE	3.3
1	D	26	LEU	3.3
1	F	46	MET	3.3
1	F	168	THR	3.3
1	D	594	GLY	3.2
1	F	115	HIS	3.2
1	E	587	GLY	3.2
1	F	233	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	165	VAL	3.2
1	D	41	LEU	3.1
1	F	184	CYS	3.1
1	F	63	LYS	3.1
1	E	158	MET	3.0
1	F	232	ALA	3.0
1	F	169	ASP	3.0
1	F	436	THR	3.0
1	C	669	ASP	3.0
1	F	177	ALA	3.0
1	F	131	PHE	3.0
1	A	185	GLU	2.9
1	F	129	ASN	2.9
1	B	445	LEU	2.9
1	B	130	LEU	2.9
1	D	187	GLU	2.9
1	C	594	GLY	2.9
1	B	105	CYS	2.9
1	C	703	ILE	2.8
1	B	103	GLN	2.8
1	C	43	GLN	2.8
1	D	157	GLY	2.8
1	D	100	ILE	2.8
1	D	770	SER	2.8
1	C	24	ASN	2.8
1	E	594	GLY	2.8
1	C	670	VAL	2.7
1	A	164	LYS	2.7
1	C	41	LEU	2.7
1	A	130	LEU	2.7
1	A	116	VAL	2.7
1	B	423	ILE	2.7
1	D	672	LEU	2.7
1	D	82	ILE	2.7
1	A	187	GLU	2.6
1	A	208	GLY	2.6
1	F	144	ARG	2.6
1	B	337	GLN	2.6
1	C	428	ASP	2.6
1	F	103	GLN	2.6
1	A	190	LYS	2.6
1	D	39	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	444	SER	2.6
1	D	173	TYR	2.6
1	E	432	LEU	2.6
1	F	188	PRO	2.5
1	D	445	LEU	2.5
1	C	668	LYS	2.5
1	A	141	GLU	2.5
1	A	193	ASP	2.5
1	F	40	SER	2.5
1	F	194	GLU	2.5
1	F	126	ILE	2.5
1	F	189	ILE	2.5
1	E	130	LEU	2.5
1	D	134	TYR	2.5
1	C	21	ASN	2.5
1	A	113	ARG	2.5
1	E	445	LEU	2.5
1	E	50	GLN	2.5
1	F	434	ASP	2.5
1	F	388	MET	2.5
1	F	71	VAL	2.5
1	D	62	LYS	2.5
1	E	233	ILE	2.5
1	A	129	ASN	2.4
1	F	109	LYS	2.4
1	C	50	GLN	2.4
1	A	166	VAL	2.4
1	A	41	LEU	2.4
1	F	128	GLY	2.4
1	F	148	LYS	2.4
1	D	46	MET	2.4
1	D	507	GLY	2.4
1	C	430	ILE	2.4
1	D	25	ARG	2.4
1	C	768	PHE	2.4
1	B	437	ILE	2.4
1	F	706	GLU	2.3
1	D	133	VAL	2.3
1	C	736	PHE	2.3
1	D	554	GLU	2.3
1	B	56	THR	2.3
1	F	460	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	188	PRO	2.2
2	U	227	ALA	2.2
1	F	114	ILE	2.2
1	D	440	GLU	2.2
1	F	99	VAL	2.2
1	A	117	LEU	2.2
1	B	460	ASN	2.2
1	D	43	GLN	2.2
1	E	117	LEU	2.2
1	C	452	PHE	2.2
1	E	672	LEU	2.2
1	D	102	ILE	2.2
1	A	51	LEU	2.2
1	D	438	ASP	2.2
2	U	230	GLY	2.2
1	F	44	PRO	2.2
1	D	506	PHE	2.2
1	F	394	VAL	2.2
1	A	237	PRO	2.2
1	B	104	PRO	2.2
1	B	452	PHE	2.2
1	A	82	ILE	2.1
1	A	433	GLU	2.1
1	E	71	VAL	2.1
1	F	428	ASP	2.1
1	D	71	VAL	2.1
1	D	729	PRO	2.1
1	F	199	ASN	2.1
1	A	175	ILE	2.1
1	E	172	PRO	2.1
1	B	336	LYS	2.1
1	F	47	ASP	2.1
1	E	736	PHE	2.1
1	B	109	LYS	2.1
1	F	147	ARG	2.1
1	F	135	LEU	2.1
1	F	429	LEU	2.0
1	E	708	ARG	2.0
1	F	24	ASN	2.0
1	D	447	VAL	2.0
1	F	138	TYR	2.0
1	D	233	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	729	PRO	2.0
1	F	42	SER	2.0
1	D	505	LYS	2.0
1	E	23	PRO	2.0
1	D	99	VAL	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(Å^2)	Q<0.9
6	GOL	F	906	6/6	0.81	0.38	<mark>5.41</mark>	108,130,150,155	0
5	CL	F	905	1/1	0.92	0.35	1.78	109,109,109,109	0
5	CL	C	901	1/1	0.71	0.31	1.47	130,130,130,130	0
3	AGS	F	902	31/31	0.92	0.28	1.40	55,88,149,575	0
5	CL	E	905	1/1	0.80	0.36	1.18	118,118,118,118	0
3	AGS	C	902	31/31	0.96	0.30	1.13	72,100,145,218	0
5	CL	D	901	1/1	0.73	0.31	0.99	117,117,117,117	0
5	CL	A	905	1/1	0.84	0.32	0.83	98,98,98,98	0
3	AGS	A	902	31/31	0.96	0.24	0.67	55,100,134,142	0
3	AGS	F	901	31/31	0.94	0.30	0.34	83,125,164,219	0
5	CL	B	905	1/1	0.89	0.28	0.32	105,105,105,105	0
3	AGS	B	902	31/31	0.95	0.23	0.27	70,99,130,144	0
3	AGS	E	902	31/31	0.94	0.23	0.26	57,97,116,136	0
3	AGS	D	903	31/31	0.96	0.23	0.16	66,97,120,134	0
3	AGS	B	901	31/31	0.97	0.24	0.10	63,101,152,169	0
6	GOL	F	907	6/6	0.94	0.24	0.03	92,114,131,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	AGS	A	901	31/31	0.96	0.29	-0.01	71,108,176,255	0
3	AGS	C	903	31/31	0.96	0.22	-0.08	79,114,143,164	0
3	AGS	D	902	31/31	0.96	0.19	-0.82	79,106,154,239	0
3	AGS	E	901	31/31	0.96	0.18	-0.91	81,106,140,164	0
4	MG	C	904	1/1	0.92	0.29	-	111,111,111,111	0
4	MG	E	904	1/1	0.95	0.33	-	100,100,100,100	0
4	MG	D	904	1/1	0.96	0.10	-	139,139,139,139	0
4	MG	B	904	1/1	0.96	0.28	-	99,99,99,99	0
4	MG	F	904	1/1	0.96	0.29	-	70,70,70,70	0
4	MG	A	904	1/1	0.98	0.29	-	86,86,86,86	0
4	MG	D	905	1/1	0.89	0.28	-	100,100,100,100	0
4	MG	E	903	1/1	0.96	0.11	-	115,115,115,115	0
4	MG	F	903	1/1	0.97	0.19	-	199,199,199,199	0
4	MG	C	905	1/1	0.97	0.25	-	102,102,102,102	0
4	MG	A	903	1/1	0.78	0.19	-	243,243,243,243	0
4	MG	B	903	1/1	0.89	0.17	-	139,139,139,139	0

6.5 Other polymers (i)

There are no such residues in this entry.