



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:51 AM UTC

PDB ID : 4LF2 / pdb_00004lf2
Title : Hexameric Form II RuBisCO from Rhodopseudomonas palustris, activated and complexed with sulfate and magnesium
Authors : Chan, S.; Satagopan, S.; Sawaya, M.R.; Eisenberg, D.; Tabita, F.R.; Perry, L.J.
Deposited on : 2013-06-26
Resolution : 2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

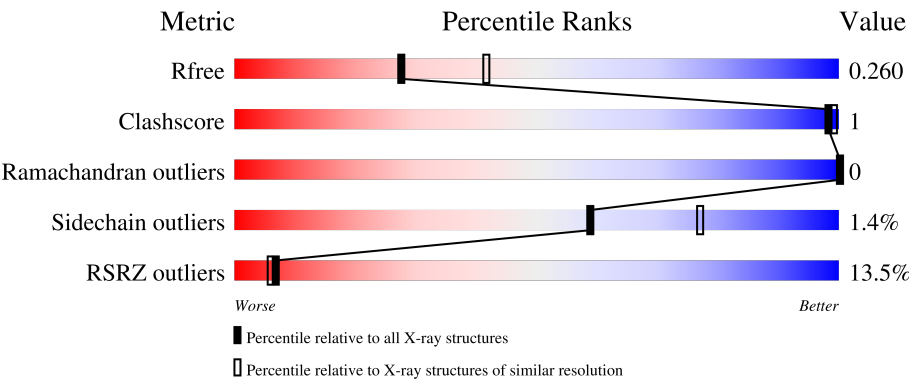
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	481	8% 93% 5%
1	B	481	12% 90% 6%
1	C	481	14% 92% 6%
1	D	481	9% 93% 5%
1	E	481	16% 92% 5%

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Mol	Chain	Length	Quality of chain
1	F	481	18% 93% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22617 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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	5	4	0
			3557	2262	614	662	19			
1	B	453	Total	C	N	O	S	3	2	0
			3514	2232	608	655	19			
1	C	453	Total	C	N	O	S	5	1	0
			3513	2231	610	653	19			
1	D	457	Total	C	N	O	S	9	0	0
			3536	2247	613	657	19			
1	E	455	Total	C	N	O	S	6	1	0
			3522	2238	610	656	18			
1	F	456	Total	C	N	O	S	8	2	0
			3537	2249	613	657	18			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q6N0W9
A	-18	GLY	-	expression tag	UNP Q6N0W9
A	-17	SER	-	expression tag	UNP Q6N0W9
A	-16	SER	-	expression tag	UNP Q6N0W9
A	-15	HIS	-	expression tag	UNP Q6N0W9
A	-14	HIS	-	expression tag	UNP Q6N0W9
A	-13	HIS	-	expression tag	UNP Q6N0W9
A	-12	HIS	-	expression tag	UNP Q6N0W9
A	-11	HIS	-	expression tag	UNP Q6N0W9
A	-10	HIS	-	expression tag	UNP Q6N0W9
A	-9	SER	-	expression tag	UNP Q6N0W9
A	-8	SER	-	expression tag	UNP Q6N0W9
A	-7	GLY	-	expression tag	UNP Q6N0W9
A	-6	LEU	-	expression tag	UNP Q6N0W9
A	-5	VAL	-	expression tag	UNP Q6N0W9
A	-4	PRO	-	expression tag	UNP Q6N0W9
A	-3	ARG	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q6N0W9
A	-1	SER	-	expression tag	UNP Q6N0W9
A	0	HIS	-	expression tag	UNP Q6N0W9
B	-19	MET	-	initiating methionine	UNP Q6N0W9
B	-18	GLY	-	expression tag	UNP Q6N0W9
B	-17	SER	-	expression tag	UNP Q6N0W9
B	-16	SER	-	expression tag	UNP Q6N0W9
B	-15	HIS	-	expression tag	UNP Q6N0W9
B	-14	HIS	-	expression tag	UNP Q6N0W9
B	-13	HIS	-	expression tag	UNP Q6N0W9
B	-12	HIS	-	expression tag	UNP Q6N0W9
B	-11	HIS	-	expression tag	UNP Q6N0W9
B	-10	HIS	-	expression tag	UNP Q6N0W9
B	-9	SER	-	expression tag	UNP Q6N0W9
B	-8	SER	-	expression tag	UNP Q6N0W9
B	-7	GLY	-	expression tag	UNP Q6N0W9
B	-6	LEU	-	expression tag	UNP Q6N0W9
B	-5	VAL	-	expression tag	UNP Q6N0W9
B	-4	PRO	-	expression tag	UNP Q6N0W9
B	-3	ARG	-	expression tag	UNP Q6N0W9
B	-2	GLY	-	expression tag	UNP Q6N0W9
B	-1	SER	-	expression tag	UNP Q6N0W9
B	0	HIS	-	expression tag	UNP Q6N0W9
C	-19	MET	-	initiating methionine	UNP Q6N0W9
C	-18	GLY	-	expression tag	UNP Q6N0W9
C	-17	SER	-	expression tag	UNP Q6N0W9
C	-16	SER	-	expression tag	UNP Q6N0W9
C	-15	HIS	-	expression tag	UNP Q6N0W9
C	-14	HIS	-	expression tag	UNP Q6N0W9
C	-13	HIS	-	expression tag	UNP Q6N0W9
C	-12	HIS	-	expression tag	UNP Q6N0W9
C	-11	HIS	-	expression tag	UNP Q6N0W9
C	-10	HIS	-	expression tag	UNP Q6N0W9
C	-9	SER	-	expression tag	UNP Q6N0W9
C	-8	SER	-	expression tag	UNP Q6N0W9
C	-7	GLY	-	expression tag	UNP Q6N0W9
C	-6	LEU	-	expression tag	UNP Q6N0W9
C	-5	VAL	-	expression tag	UNP Q6N0W9
C	-4	PRO	-	expression tag	UNP Q6N0W9
C	-3	ARG	-	expression tag	UNP Q6N0W9
C	-2	GLY	-	expression tag	UNP Q6N0W9
C	-1	SER	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q6N0W9
D	-19	MET	-	initiating methionine	UNP Q6N0W9
D	-18	GLY	-	expression tag	UNP Q6N0W9
D	-17	SER	-	expression tag	UNP Q6N0W9
D	-16	SER	-	expression tag	UNP Q6N0W9
D	-15	HIS	-	expression tag	UNP Q6N0W9
D	-14	HIS	-	expression tag	UNP Q6N0W9
D	-13	HIS	-	expression tag	UNP Q6N0W9
D	-12	HIS	-	expression tag	UNP Q6N0W9
D	-11	HIS	-	expression tag	UNP Q6N0W9
D	-10	HIS	-	expression tag	UNP Q6N0W9
D	-9	SER	-	expression tag	UNP Q6N0W9
D	-8	SER	-	expression tag	UNP Q6N0W9
D	-7	GLY	-	expression tag	UNP Q6N0W9
D	-6	LEU	-	expression tag	UNP Q6N0W9
D	-5	VAL	-	expression tag	UNP Q6N0W9
D	-4	PRO	-	expression tag	UNP Q6N0W9
D	-3	ARG	-	expression tag	UNP Q6N0W9
D	-2	GLY	-	expression tag	UNP Q6N0W9
D	-1	SER	-	expression tag	UNP Q6N0W9
D	0	HIS	-	expression tag	UNP Q6N0W9
E	-19	MET	-	initiating methionine	UNP Q6N0W9
E	-18	GLY	-	expression tag	UNP Q6N0W9
E	-17	SER	-	expression tag	UNP Q6N0W9
E	-16	SER	-	expression tag	UNP Q6N0W9
E	-15	HIS	-	expression tag	UNP Q6N0W9
E	-14	HIS	-	expression tag	UNP Q6N0W9
E	-13	HIS	-	expression tag	UNP Q6N0W9
E	-12	HIS	-	expression tag	UNP Q6N0W9
E	-11	HIS	-	expression tag	UNP Q6N0W9
E	-10	HIS	-	expression tag	UNP Q6N0W9
E	-9	SER	-	expression tag	UNP Q6N0W9
E	-8	SER	-	expression tag	UNP Q6N0W9
E	-7	GLY	-	expression tag	UNP Q6N0W9
E	-6	LEU	-	expression tag	UNP Q6N0W9
E	-5	VAL	-	expression tag	UNP Q6N0W9
E	-4	PRO	-	expression tag	UNP Q6N0W9
E	-3	ARG	-	expression tag	UNP Q6N0W9
E	-2	GLY	-	expression tag	UNP Q6N0W9
E	-1	SER	-	expression tag	UNP Q6N0W9
E	0	HIS	-	expression tag	UNP Q6N0W9
F	-19	MET	-	initiating methionine	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP Q6N0W9
F	-17	SER	-	expression tag	UNP Q6N0W9
F	-16	SER	-	expression tag	UNP Q6N0W9
F	-15	HIS	-	expression tag	UNP Q6N0W9
F	-14	HIS	-	expression tag	UNP Q6N0W9
F	-13	HIS	-	expression tag	UNP Q6N0W9
F	-12	HIS	-	expression tag	UNP Q6N0W9
F	-11	HIS	-	expression tag	UNP Q6N0W9
F	-10	HIS	-	expression tag	UNP Q6N0W9
F	-9	SER	-	expression tag	UNP Q6N0W9
F	-8	SER	-	expression tag	UNP Q6N0W9
F	-7	GLY	-	expression tag	UNP Q6N0W9
F	-6	LEU	-	expression tag	UNP Q6N0W9
F	-5	VAL	-	expression tag	UNP Q6N0W9
F	-4	PRO	-	expression tag	UNP Q6N0W9
F	-3	ARG	-	expression tag	UNP Q6N0W9
F	-2	GLY	-	expression tag	UNP Q6N0W9
F	-1	SER	-	expression tag	UNP Q6N0W9
F	0	HIS	-	expression tag	UNP Q6N0W9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

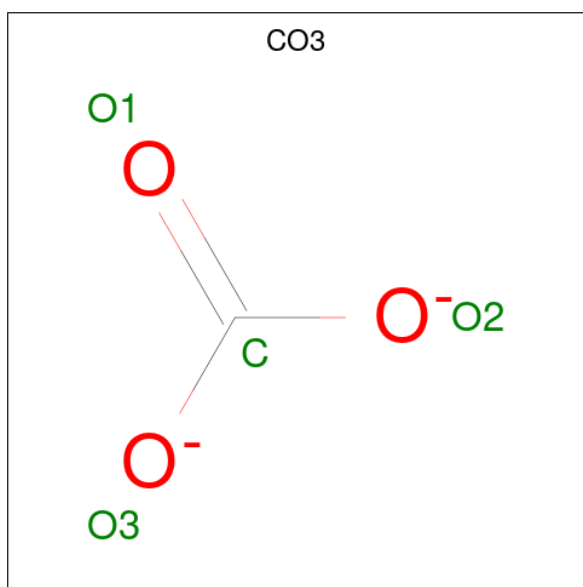
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



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

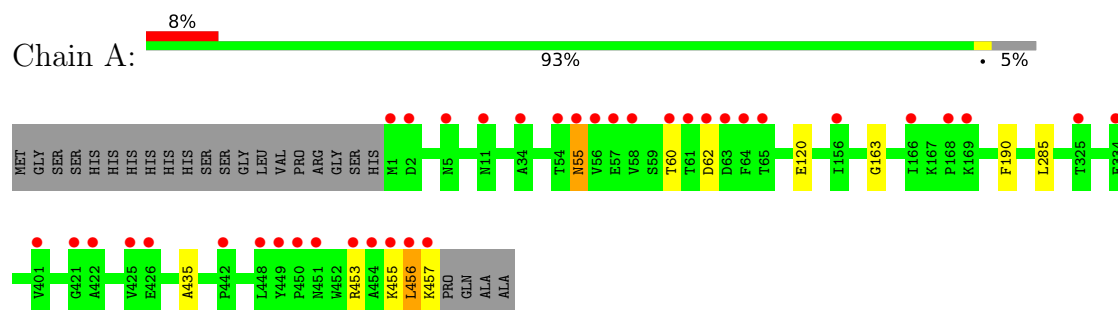
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total	O	0	0
			239	239		
5	B	243	Total	O	0	0
			243	243		
5	C	254	Total	O	0	0
			254	254		
5	D	245	Total	O	0	0
			245	245		
5	E	197	Total	O	0	0
			197	197		
5	F	184	Total	O	0	0
			184	184		

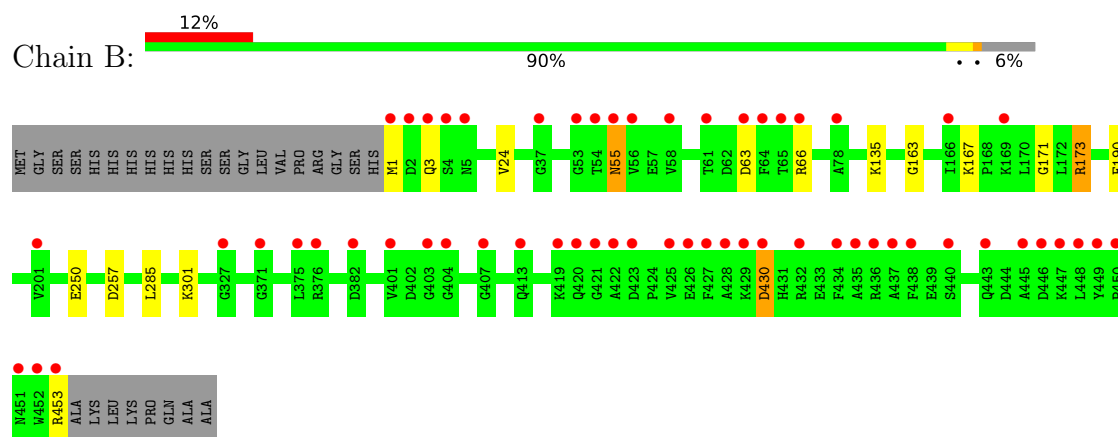
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

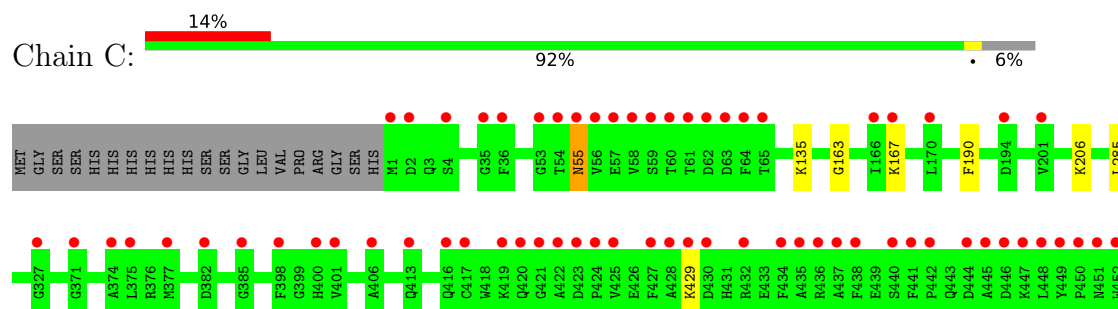
- Molecule 1: Ribulose biphosphate carboxylase

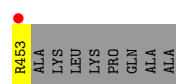


- Molecule 1: Ribulose biphosphate carboxylase



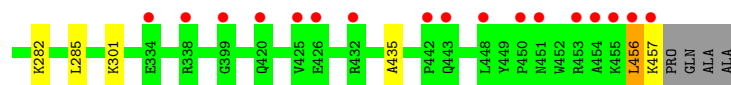
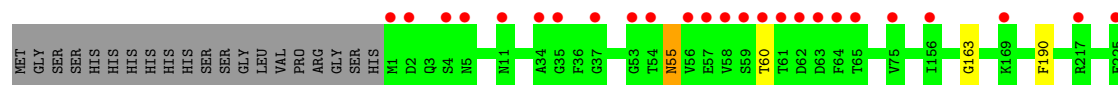
- Molecule 1: Ribulose biphosphate carboxylase





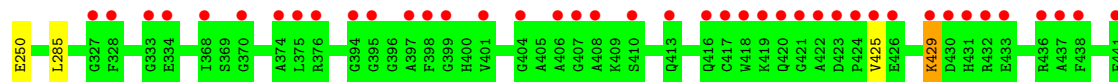
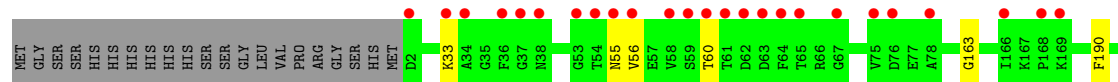
- Molecule 1: Ribulose biphosphate carboxylase

Chain D: 9% 93% 5%



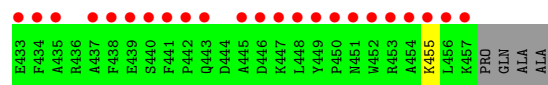
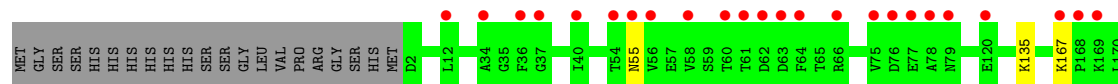
- Molecule 1: Ribulose biphosphate carboxylase

Chain E: 16% 92% 5%



- Molecule 1: Ribulose biphosphate carboxylase

Chain F: 18% 93% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.22Å 99.78Å 100.00Å 67.30° 71.28° 86.63°	Depositor
Resolution (Å)	87.43 – 2.38 87.43 – 2.38	Depositor EDS
% Data completeness (in resolution range)	96.6 (87.43-2.38) 96.6 (87.43-2.38)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.86Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.258 0.207 , 0.260	Depositor DCC
R_{free} test set	7318 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtrriage
Anisotropy	0.156	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22617	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4135e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, KCX, MG, CO3

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	0.80	0/3645	1.01	2/4929 (0.0%)
1	B	0.81	0/3596	1.01	2/4866 (0.0%)
1	C	0.82	1/3592 (0.0%)	1.00	1/4860 (0.0%)
1	D	0.80	0/3612	0.99	1/4886 (0.0%)
1	E	0.81	0/3601	1.01	1/4873 (0.0%)
1	F	0.82	0/3619	1.01	0/4895
All	All	0.81	1/21665 (0.0%)	1.00	7/29309 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	429	LYS	CG-CD	5.45	1.68	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	455	LYS	N-CA-C	6.36	119.51	111.69
1	A	453	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	B	55	ASN	N-CA-C	5.24	119.30	113.01
1	C	55	ASN	N-CA-C	5.20	119.25	113.01
1	D	55	ASN	N-CA-C	5.14	119.18	113.01
1	A	55	ASN	N-CA-C	5.14	119.17	113.01
1	B	24	VAL	N-CA-C	-5.10	102.27	109.21

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	3557	0	3444	4	0
1	B	3514	0	3385	10	0
1	C	3513	0	3385	4	0
1	D	3536	0	3414	4	0
1	E	3522	0	3394	5	0
1	F	3537	0	3420	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
5	A	239	0	0	0	0
5	B	243	0	0	2	0
5	C	254	0	0	0	0
5	D	245	0	0	1	0
5	E	197	0	0	0	0
5	F	184	0	0	2	0
All	All	22617	0	20442	24	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (24) 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:3[B]:GLN:HE21	1:B:3[B]:GLN:HA	1.62	0.64
1:A:62:ASP:OD2	1:B:173:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LYS:NZ	5:B:784:HOH:O	2.33	0.62
1:D:301:LYS:NZ	5:D:935:HOH:O	2.33	0.59
1:E:425:VAL:O	1:E:429:LYS:NZ	2.38	0.56
1:E:56:VAL:HG11	1:F:395:GLY:HA3	1.88	0.54
1:F:135:LYS:NZ	5:F:902:HOH:O	2.43	0.51
1:A:435:ALA:HB1	1:A:456:LEU:HD21	1.96	0.47
1:A:60:THR:OG1	1:B:167:LYS:O	2.22	0.46
1:C:167:LYS:O	1:D:60:THR:OG1	2.23	0.46
1:E:60:THR:OG1	1:F:167:LYS:O	2.26	0.45
1:B:301:LYS:NZ	5:B:767:HOH:O	2.34	0.45
1:B:430:ASP:OD1	1:B:430:ASP:N	2.51	0.44
1:F:322:HIS:ND1	5:F:904:HOH:O	2.32	0.43
1:A:163:GLY:HA2	1:A:190:PHE:O	2.20	0.42
1:B:171:GLY:O	1:B:173:ARG:NH1	2.52	0.42
1:D:163:GLY:HA2	1:D:190:PHE:O	2.20	0.42
1:B:63:ASP:OD1	1:B:66:ARG:NH1	2.53	0.42
1:D:435:ALA:HB1	1:D:456:LEU:HD21	2.01	0.41
1:B:163:GLY:HA2	1:B:190:PHE:O	2.21	0.41
1:C:163:GLY:HA2	1:C:190:PHE:O	2.21	0.41
1:E:163:GLY:HA2	1:E:190:PHE:O	2.21	0.41
1:B:257:ASP:OD2	1:C:135:LYS:NZ	2.47	0.40
1:C:206:LYS:NZ	1:E:250:GLU:OE2	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/481 (95%)	447 (98%)	11 (2%)	0	100	100
1	B	452/481 (94%)	442 (98%)	10 (2%)	0	100	100
1	C	451/481 (94%)	442 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	454/481 (94%)	444 (98%)	10 (2%)	0	100	100
1	E	453/481 (94%)	441 (97%)	12 (3%)	0	100	100
1	F	455/481 (95%)	443 (97%)	12 (3%)	0	100	100
All	All	2723/2886 (94%)	2659 (98%)	64 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/372 (96%)	351 (98%)	6 (2%)	53	72
1	B	352/372 (95%)	345 (98%)	7 (2%)	48	68
1	C	351/372 (94%)	348 (99%)	3 (1%)	70	84
1	D	353/372 (95%)	348 (99%)	5 (1%)	59	77
1	E	352/372 (95%)	347 (99%)	5 (1%)	59	77
1	F	354/372 (95%)	351 (99%)	3 (1%)	73	85
All	All	2119/2232 (95%)	2090 (99%)	29 (1%)	59	77

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	120	GLU
1	A	285	LEU
1	A	455	LYS
1	A	456	LEU
1	A	457	LYS
1	B	1	MET
1	B	55	ASN
1	B	173	ARG
1	B	250	GLU

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Mol	Chain	Res	Type
1	B	285	LEU
1	B	430	ASP
1	B	453	ARG
1	C	55	ASN
1	C	285	LEU
1	C	453	ARG
1	D	55	ASN
1	D	282	LYS
1	D	285	LEU
1	D	456	LEU
1	D	457	LYS
1	E	33	LYS
1	E	55	ASN
1	E	285	LEU
1	E	429	LYS
1	E	451	ASN
1	F	55	ASN
1	F	285	LEU
1	F	455	LYS

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

Mol	Chain	Res	Type
1	E	79	ASN
1	F	451	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	E	192	1	10,11,12	0.52	0	6,12,14	0.51	0
1	KCX	A	192	2,1	10,11,12	0.56	0	6,12,14	0.50	0
1	KCX	C	192	1	10,11,12	0.51	0	6,12,14	0.48	0
1	KCX	B	192	2,1	10,11,12	0.51	0	6,12,14	0.53	0
1	KCX	D	192	2,1	10,11,12	0.56	0	6,12,14	0.49	0
1	KCX	F	192	1	10,11,12	0.61	0	6,12,14	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	E	192	1	-	0/9/10/12	-
1	KCX	A	192	2,1	-	0/9/10/12	-
1	KCX	C	192	1	-	0/9/10/12	-
1	KCX	B	192	2,1	-	0/9/10/12	-
1	KCX	D	192	2,1	-	0/9/10/12	-
1	KCX	F	192	1	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	SO4	D	603	-	4,4,4	0.39	0	6,6,6	0.10	0
3	SO4	E	701	-	4,4,4	0.39	0	6,6,6	0.32	0
3	SO4	A	603	-	4,4,4	0.41	0	6,6,6	0.21	0
3	SO4	C	602	-	4,4,4	0.45	0	6,6,6	0.41	0
3	SO4	B	602	-	4,4,4	0.40	0	6,6,6	0.35	0
3	SO4	D	602	-	4,4,4	0.38	0	6,6,6	0.58	0
3	SO4	B	603	-	4,4,4	0.40	0	6,6,6	0.26	0
4	CO3	A	604	-	3,3,3	1.13	0	2,3,3	0.15	0
3	SO4	A	602	-	4,4,4	0.46	0	6,6,6	0.50	0
4	CO3	C	604	-	3,3,3	1.10	0	2,3,3	0.23	0
3	SO4	F	701	-	4,4,4	0.33	0	6,6,6	0.49	0
3	SO4	F	702	-	4,4,4	0.42	0	6,6,6	0.08	0
4	CO3	B	604	-	3,3,3	1.13	0	2,3,3	0.14	0
3	SO4	C	603	-	4,4,4	0.42	0	6,6,6	0.11	0
3	SO4	E	702	-	4,4,4	0.37	0	6,6,6	0.13	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 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	456/481 (94%)	0.51	37 (8%)	18 16	4, 17, 54, 90	6 (1%)
1	B	452/481 (93%)	0.72	58 (12%)	7 7	5, 16, 61, 92	3 (0%)
1	C	452/481 (93%)	0.75	67 (14%)	5 5	4, 16, 61, 102	3 (0%)
1	D	456/481 (94%)	0.53	42 (9%)	14 13	4, 16, 50, 130	6 (1%)
1	E	454/481 (94%)	0.95	78 (17%)	4 3	4, 21, 74, 122	3 (0%)
1	F	455/481 (94%)	0.95	85 (18%)	3 3	5, 21, 69, 112	5 (1%)
All	All	2725/2886 (94%)	0.73	367 (13%)	7 6	4, 18, 63, 130	26 (0%)

All (367) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	401	VAL	6.7
1	C	450	PRO	6.7
1	D	61	THR	6.6
1	B	448	LEU	6.6
1	F	401	VAL	6.5
1	F	437	ALA	6.3
1	F	448	LEU	5.9
1	F	456	LEU	5.9
1	C	434	PHE	5.8
1	D	454	ALA	5.7
1	B	58	VAL	5.7
1	E	399	GLY	5.7
1	E	448	LEU	5.7
1	D	62	ASP	5.6
1	A	454	ALA	5.4
1	D	451	ASN	5.4
1	A	61	THR	5.3
1	C	435	ALA	5.1
1	D	456	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	440	SER	5.1
1	C	375	LEU	5.0
1	F	449	TYR	5.0
1	E	437	ALA	4.8
1	F	399	GLY	4.8
1	C	420	GLN	4.7
1	B	53	GLY	4.7
1	D	54	THR	4.6
1	F	451	ASN	4.6
1	B	64	PHE	4.5
1	E	60	THR	4.5
1	B	425	VAL	4.5
1	E	54	THR	4.4
1	F	450	PRO	4.4
1	E	456	LEU	4.4
1	C	2	ASP	4.4
1	E	63	ASP	4.4
1	E	454	ALA	4.4
1	F	425	VAL	4.4
1	D	63	ASP	4.3
1	E	421	GLY	4.3
1	C	451	ASN	4.3
1	F	441	PHE	4.3
1	F	370	GLY	4.3
1	F	56	VAL	4.2
1	A	169	LYS	4.2
1	F	454	ALA	4.2
1	B	434	PHE	4.2
1	D	64	PHE	4.2
1	A	58	VAL	4.1
1	E	374	ALA	4.1
1	E	61	THR	4.0
1	F	447	LYS	3.9
1	A	421	GLY	3.9
1	E	426	GLU	3.9
1	E	53	GLY	3.9
1	F	395	GLY	3.9
1	D	420	GLN	3.9
1	D	457	LYS	3.9
1	F	438	PHE	3.9
1	A	56	VAL	3.9
1	B	56	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	422	ALA	3.8
1	C	445	ALA	3.8
1	B	55	ASN	3.8
1	C	424	PRO	3.8
1	B	420	GLN	3.8
1	E	64	PHE	3.8
1	C	327	GLY	3.8
1	F	424	PRO	3.7
1	E	418	TRP	3.7
1	C	421	GLY	3.7
1	E	420	GLN	3.7
1	F	434	PHE	3.7
1	E	447	LYS	3.7
1	E	425	VAL	3.7
1	B	449	TYR	3.7
1	A	456	LEU	3.7
1	F	37	GLY	3.7
1	A	62	ASP	3.6
1	E	55	ASN	3.6
1	B	54	THR	3.6
1	D	59	SER	3.6
1	F	430	ASP	3.6
1	F	61	THR	3.6
1	F	455	LYS	3.6
1	C	423	ASP	3.6
1	E	406	ALA	3.6
1	F	457	LYS	3.5
1	B	166	ILE	3.5
1	E	370	GLY	3.5
1	C	452	TRP	3.5
1	C	371	GLY	3.5
1	F	446	ASP	3.5
1	F	60	THR	3.5
1	F	442	PRO	3.5
1	D	455	LYS	3.5
1	B	423	ASP	3.5
1	B	451	ASN	3.5
1	E	37	GLY	3.4
1	A	64	PHE	3.4
1	F	421	GLY	3.4
1	D	60	THR	3.4
1	B	426	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	448	LEU	3.4
1	E	445	ALA	3.4
1	F	435	ALA	3.4
1	A	60	THR	3.3
1	B	401	VAL	3.3
1	B	327	GLY	3.3
1	D	1	MET	3.3
1	B	435	ALA	3.2
1	C	447	LYS	3.2
1	F	168	PRO	3.2
1	E	449	TYR	3.2
1	E	56	VAL	3.2
1	B	5	ASN	3.2
1	B	446	ASP	3.2
1	F	63	ASP	3.2
1	F	169	LYS	3.2
1	E	417	CYS	3.2
1	C	441	PHE	3.2
1	E	376	ARG	3.2
1	C	425	VAL	3.2
1	C	166	ILE	3.2
1	A	54	THR	3.2
1	C	53	GLY	3.2
1	D	56	VAL	3.2
1	E	58	VAL	3.2
1	A	448	LEU	3.2
1	B	428	ALA	3.1
1	E	166	ILE	3.1
1	C	438	PHE	3.1
1	B	2	ASP	3.1
1	B	419	LYS	3.1
1	D	156	ILE	3.1
1	E	423	ASP	3.1
1	C	422	ALA	3.1
1	B	201	VAL	3.1
1	B	450	PRO	3.1
1	A	1	MET	3.1
1	C	1	MET	3.1
1	B	63	ASP	3.1
1	C	437	ALA	3.1
1	E	78	ALA	3.1
1	E	422	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	375	LEU	3.1
1	B	452	TRP	3.0
1	E	59	SER	3.0
1	C	427	PHE	3.0
1	D	5	ASN	3.0
1	E	446	ASP	3.0
1	B	4	SER	3.0
1	C	59	SER	3.0
1	E	327	GLY	3.0
1	F	402	ASP	3.0
1	C	36	PHE	3.0
1	D	65	THR	3.0
1	E	2	ASP	3.0
1	F	398	PHE	3.0
1	F	427	PHE	3.0
1	C	417	CYS	3.0
1	C	56	VAL	3.0
1	D	450	PRO	3.0
1	E	168	PRO	3.0
1	F	406	ALA	2.9
1	F	420	GLN	2.9
1	C	4	SER	2.9
1	F	410	SER	2.9
1	F	440	SER	2.9
1	D	37	GLY	2.9
1	E	62	ASP	2.9
1	E	451	ASN	2.9
1	F	452	TRP	2.9
1	B	445	ALA	2.9
1	D	432	ARG	2.9
1	A	426	GLU	2.9
1	A	451	ASN	2.9
1	A	450	PRO	2.9
1	E	424	PRO	2.9
1	D	448	LEU	2.9
1	E	438	PHE	2.9
1	E	401	VAL	2.9
1	F	75	VAL	2.9
1	D	426	GLU	2.9
1	E	34	ALA	2.9
1	D	334	GLU	2.9
1	E	444	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	62	ASP	2.9
1	F	194	ASP	2.9
1	E	404	GLY	2.8
1	F	66	ARG	2.8
1	F	34	ALA	2.8
1	F	397	ALA	2.8
1	A	425	VAL	2.8
1	F	417	CYS	2.8
1	B	429	LYS	2.8
1	A	34	ALA	2.8
1	A	57	GLU	2.8
1	B	1	MET	2.8
1	C	430	ASP	2.8
1	A	422	ALA	2.8
1	C	64	PHE	2.8
1	A	457	LYS	2.8
1	A	401	VAL	2.8
1	C	54	THR	2.8
1	A	63	ASP	2.8
1	B	447	LYS	2.8
1	C	429	LYS	2.8
1	E	397	ALA	2.8
1	F	328	PHE	2.8
1	B	453	ARG	2.8
1	F	54	THR	2.7
1	F	120	GLU	2.7
1	C	406	ALA	2.7
1	E	398	PHE	2.7
1	D	2	ASP	2.7
1	E	429	LYS	2.7
1	F	418	TRP	2.7
1	F	36	PHE	2.7
1	C	60	THR	2.7
1	E	76	ASP	2.7
1	E	334	GLU	2.7
1	B	66	ARG	2.7
1	E	375	LEU	2.7
1	C	374	ALA	2.7
1	D	58	VAL	2.7
1	C	35	GLY	2.7
1	F	375	LEU	2.7
1	F	334	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	61	THR	2.6
1	B	432	ARG	2.6
1	C	416	GLN	2.6
1	E	430	ASP	2.6
1	F	64	PHE	2.6
1	D	425	VAL	2.6
1	F	58	VAL	2.6
1	B	407	GLY	2.6
1	C	413	GLN	2.6
1	F	12	LEU	2.6
1	E	455	LYS	2.6
1	C	57	GLU	2.6
1	F	408	ALA	2.6
1	D	217	ARG	2.6
1	C	385	GLY	2.6
1	E	395	GLY	2.6
1	E	436	ARG	2.6
1	F	376	ARG	2.6
1	F	371	GLY	2.6
1	C	449	TYR	2.6
1	F	369	SER	2.6
1	F	400	HIS	2.6
1	C	444	ASP	2.5
1	D	11	ASN	2.5
1	E	38	ASN	2.5
1	A	168	PRO	2.5
1	C	201	VAL	2.5
1	E	33	LYS	2.5
1	E	368	ILE	2.5
1	E	416	GLN	2.5
1	C	453	ARG	2.5
1	C	382	ASP	2.5
1	F	445	ALA	2.5
1	E	441	PHE	2.5
1	C	58	VAL	2.5
1	D	453	ARG	2.5
1	C	194	ASP	2.5
1	C	446	ASP	2.5
1	D	34	ALA	2.5
1	B	404	GLY	2.5
1	E	67	GLY	2.5
1	E	75	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	77	GLU	2.5
1	F	432	ARG	2.5
1	C	377	MET	2.5
1	B	437	ALA	2.5
1	B	371	GLY	2.5
1	F	327	GLY	2.5
1	F	416	GLN	2.5
1	E	453	ARG	2.4
1	B	427	PHE	2.4
1	D	75	VAL	2.4
1	A	449	TYR	2.4
1	C	55	ASN	2.4
1	B	403	GLY	2.4
1	E	450	PRO	2.4
1	E	410	SER	2.4
1	C	398	PHE	2.4
1	C	170	LEU	2.4
1	E	413	GLN	2.4
1	F	76	ASP	2.4
1	F	453	ARG	2.4
1	D	35	GLY	2.4
1	E	407	GLY	2.4
1	A	5	ASN	2.4
1	D	53	GLY	2.4
1	A	166	ILE	2.4
1	A	453	ARG	2.4
1	B	37	GLY	2.3
1	E	408	ALA	2.3
1	C	65	THR	2.3
1	F	40	ILE	2.3
1	F	426	GLU	2.3
1	A	2	ASP	2.3
1	B	421	GLY	2.3
1	C	400	HIS	2.3
1	B	169	LYS	2.3
1	D	169	LYS	2.3
1	A	65	THR	2.3
1	C	436	ARG	2.3
1	B	413	GLN	2.3
1	D	225	GLU	2.3
1	D	443	GLN	2.3
1	F	411	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	55	ASN	2.3
1	B	436	ARG	2.3
1	C	428	ALA	2.3
1	D	338	ARG	2.3
1	B	65	THR	2.3
1	C	419	LYS	2.3
1	F	380	PHE	2.2
1	B	430	ASP	2.2
1	D	399	GLY	2.2
1	F	374	ALA	2.2
1	E	65	THR	2.2
1	B	376	ARG	2.2
1	F	78	ALA	2.2
1	B	443	GLN	2.2
1	E	431	HIS	2.2
1	F	443	GLN	2.2
1	B	78	ALA	2.2
1	A	455	LYS	2.2
1	C	63	ASP	2.1
1	E	169	LYS	2.1
1	B	3[A]	GLN	2.1
1	F	171	GLY	2.1
1	C	432	ARG	2.1
1	A	156	ILE	2.1
1	B	382	ASP	2.1
1	E	433	GLU	2.1
1	D	442	PRO	2.1
1	E	36	PHE	2.1
1	E	394	GLY	2.1
1	E	432	ARG	2.1
1	F	167	LYS	2.1
1	F	331	MET	2.1
1	F	373	ASN	2.1
1	A	442	PRO	2.1
1	B	438	PHE	2.1
1	F	333	GLY	2.1
1	C	61	THR	2.1
1	C	62	ASP	2.1
1	E	328	PHE	2.1
1	C	167	LYS	2.0
1	A	325	THR	2.0
1	B	440	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	334[A]	GLU	2.0
1	D	57	GLU	2.0
1	F	336	ALA	2.0
1	A	55	ASN	2.0
1	F	79	ASN	2.0
1	E	333	GLY	2.0
1	D	4	SER	2.0
1	F	433	GLU	2.0
1	F	439	GLU	2.0
1	A	11	ASN	2.0
1	C	442	PRO	2.0
1	E	419	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KCX	B	192	12/13	0.88	0.13	14,25,34,48	0
1	KCX	C	192	12/13	0.90	0.10	13,22,36,52	0
1	KCX	D	192	12/13	0.90	0.10	15,18,28,31	0
1	KCX	F	192	12/13	0.90	0.10	16,25,45,53	0
1	KCX	E	192	12/13	0.91	0.10	11,17,36,42	0
1	KCX	A	192	12/13	0.92	0.08	11,17,26,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	C	601	1/1	0.77	0.12	52,52,52,52	0
4	CO3	C	604	4/4	0.81	0.14	28,31,46,64	0
3	SO4	B	602	5/5	0.86	0.13	18,29,42,53	0
2	MG	B	601	1/1	0.87	0.13	62,62,62,62	0
3	SO4	C	602	5/5	0.87	0.12	15,31,34,44	0
3	SO4	E	701	5/5	0.87	0.15	25,37,47,72	0
3	SO4	F	702	5/5	0.87	0.11	39,51,62,70	0
2	MG	A	601	1/1	0.87	0.07	34,34,34,34	0
3	SO4	A	602	5/5	0.88	0.14	15,19,39,44	0
4	CO3	B	604	4/4	0.88	0.11	37,38,40,70	0
3	SO4	F	701	5/5	0.88	0.14	35,38,45,63	0
4	CO3	A	604	4/4	0.89	0.10	29,43,50,57	0
3	SO4	C	603	5/5	0.90	0.11	42,43,59,79	0
3	SO4	E	702	5/5	0.91	0.12	39,44,50,52	0
3	SO4	D	602	5/5	0.91	0.11	15,23,46,47	0
3	SO4	B	603	5/5	0.93	0.15	29,36,44,56	0
2	MG	D	601	1/1	0.95	0.06	44,44,44,44	0
3	SO4	A	603	5/5	0.98	0.06	17,29,32,35	0
3	SO4	D	603	5/5	0.99	0.07	18,24,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.