



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:12 AM UTC

PDB ID : 6FAD / pdb_00006fad
Title : SR protein kinase 1 (SRPK1) in complex with the RGG-box of HSV1 ICP27
Authors : Tunncliffe, R.B.; Levy, C.; Mould, A.P.; Mckenzie, E.A.; Sandri-Goldin, R.M.; Golovanov, A.P.
Deposited on : 2017-12-15
Resolution : 2.80 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

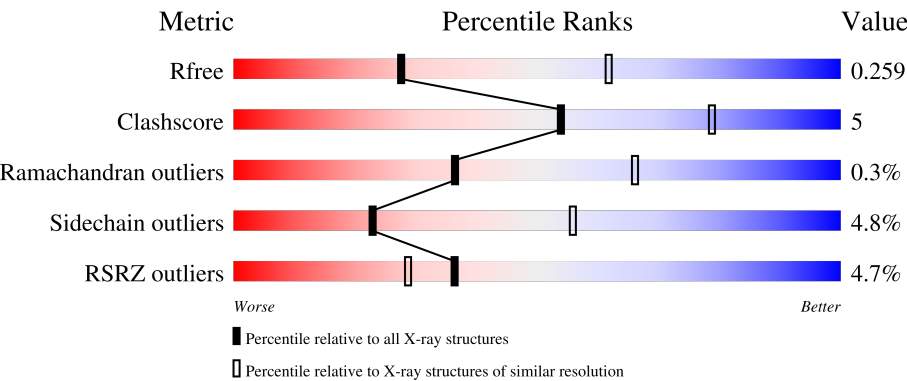
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	618	2% 51%6%42%
1	B	618	3% 49%8%42%
1	C	618	3% 47%11%42%
1	D	618	2% 48%9%42%
2	E	16	12% 56%19%25%

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Mol	Chain	Length	Quality of chain
2	F	16	6% 38% 6% 56%
2	G	16	6% 38% 6% 6% 50%
2	H	16	31% 50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12099 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 SRSF protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2892	1868	493	519	12			
1	B	356	Total	C	N	O	S	0	0	0
			2892	1868	493	519	12			
1	C	359	Total	C	N	O	S	0	0	0
			2915	1883	497	523	12			
1	D	356	Total	C	N	O	S	0	0	0
			2892	1868	493	519	12			

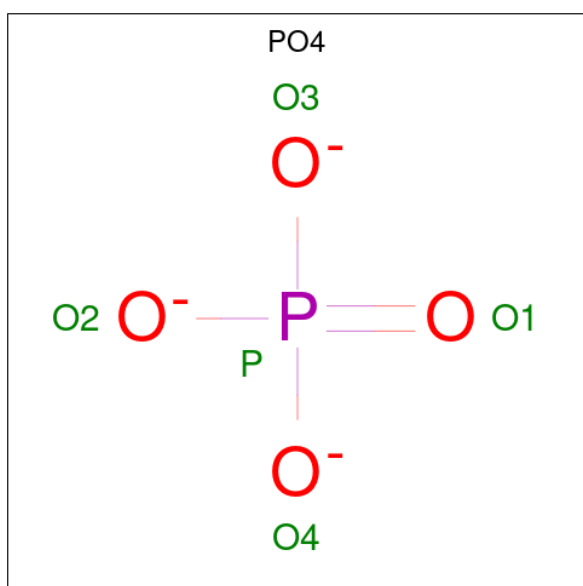
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLY	-	expression tag	UNP Q96SB4
A	39	SER	-	expression tag	UNP Q96SB4
A	40	HIS	-	expression tag	UNP Q96SB4
A	41	MET	-	expression tag	UNP Q96SB4
B	38	GLY	-	expression tag	UNP Q96SB4
B	39	SER	-	expression tag	UNP Q96SB4
B	40	HIS	-	expression tag	UNP Q96SB4
B	41	MET	-	expression tag	UNP Q96SB4
C	38	GLY	-	expression tag	UNP Q96SB4
C	39	SER	-	expression tag	UNP Q96SB4
C	40	HIS	-	expression tag	UNP Q96SB4
C	41	MET	-	expression tag	UNP Q96SB4
D	38	GLY	-	expression tag	UNP Q96SB4
D	39	SER	-	expression tag	UNP Q96SB4
D	40	HIS	-	expression tag	UNP Q96SB4
D	41	MET	-	expression tag	UNP Q96SB4

- Molecule 2 is a protein called mRNA export factor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	0	0	0
			97	52	33	12			
2	F	7	Total	C	N	O	0	0	0
			63	34	22	7			
2	G	8	Total	C	N	O	0	0	0
			67	36	23	8			
2	H	8	Total	C	N	O	0	0	0
			67	36	23	8			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

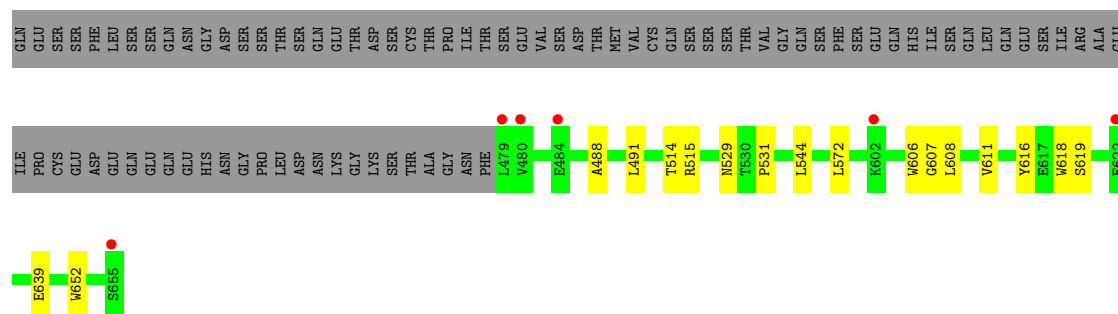
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		

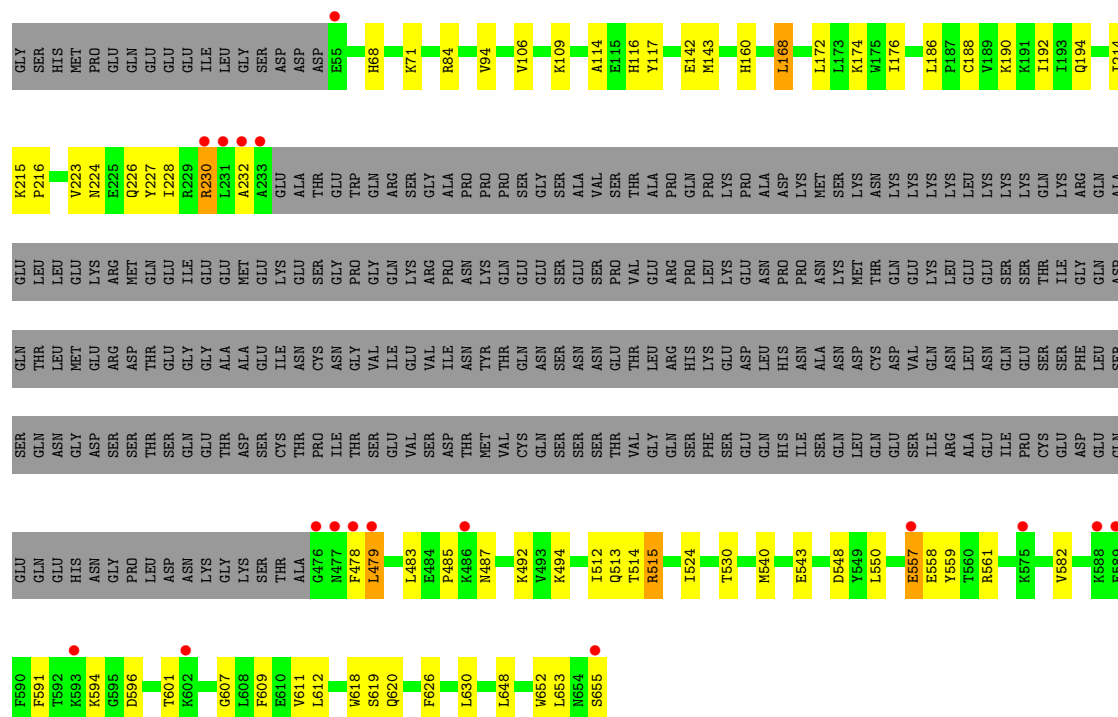
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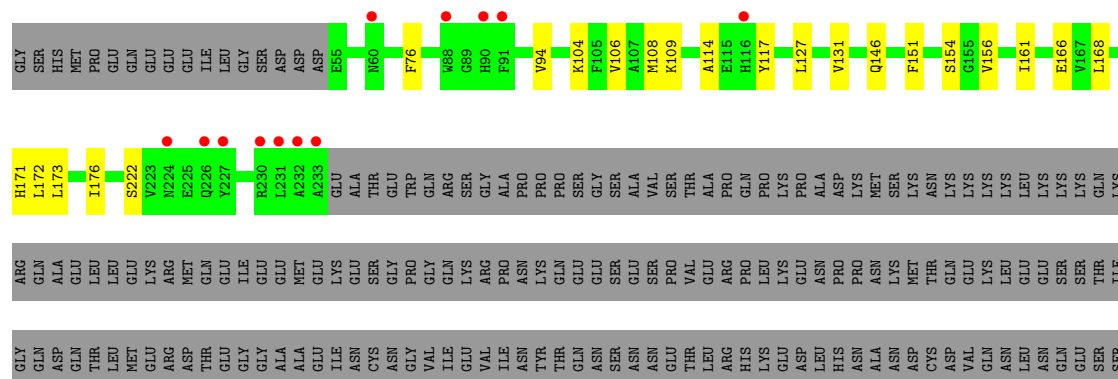
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	53	Total 53	O 53	0	0
4	C	29	Total 29	O 29	0	0
4	D	60	Total 60	O 60	0	0
4	E	2	Total 2	O 2	0	0
4	H	2	Total 2	O 2	0	0



• Molecule 1: SRSF protein kinase 1



• Molecule 1: SRSF protein kinase 1



PHE LEU SER SER LYS ASN GLY ASP ASP SER SER THR THR SER GLN GLU THR ASP CYS THR PRO ILE THR SER VAL VAL SER ASP THR MET VAL CYS GLN SER SER THR THR VAL GLY GLN SER PHE PHE SER GLU HIS ILE SER GLN LEU GLN GLU SER ILE ARG ALA GLU PRO CYS GLU

ASP GLU GLN GLN GLN HIS ASN ASN GLY SER PRO THR ASP ASP LYS GLY LYS THR THR ALA GLY ASN PHE L479 E484 E485 K486 K490 L491 K492 D497 L498 D511 Y517 N529 T530 P531 F542 E543 T546 L550 F551 E558 Y559 E563 A567 E571

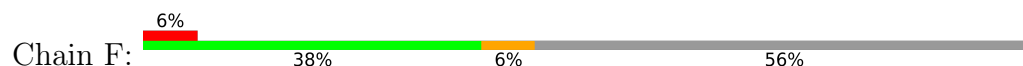
P577 R578 K579 L580 I581 V582 K588 E589 F590 K594 K602 E610 Y616 E621 L630 M633 I634 E635 L636 I637 R641 S655

• Molecule 2: mRNA export factor



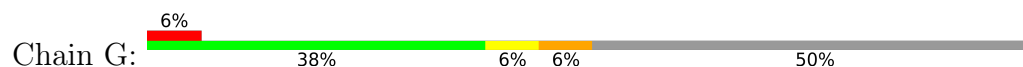
ALA R136 R146 G147 R148 G149 ARG GLY GLY

• Molecule 2: mRNA export factor



ALA ARG GLY GLY ARG R142 R143 R148 GLY ARG GLY GLY

• Molecule 2: mRNA export factor



ALA ARG GLY GLY ARG R142 G143 R144 R145 G149 ARG GLY GLY

• Molecule 2: mRNA export factor



ALA ARG GLY GLY ARG R142 R145 R146 G147 R148 G149 ARG GLY GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	99.98Å 99.98Å 426.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.21 – 2.80 80.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.21-2.80) 100.0 (80.21-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.198 , 0.257 0.201 , 0.259	Depositor DCC
R_{free} test set	2994 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12099	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.38	0/2964	0.59	0/4012
1	B	0.36	0/2964	0.56	0/4012
1	C	0.35	0/2988	0.54	0/4044
1	D	0.37	0/2964	0.56	0/4012
2	E	0.45	0/96	0.80	0/120
2	F	0.43	0/62	0.72	0/77
2	G	0.39	0/66	0.66	0/82
2	H	0.53	0/66	0.70	0/82
All	All	0.37	0/12170	0.57	0/16441

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2892	0	2905	26	0
1	B	2892	0	2904	26	0
1	C	2915	0	2921	36	0
1	D	2892	0	2905	30	0
2	E	97	0	105	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	63	0	70	1	0
2	G	67	0	73	2	0
2	H	67	0	73	0	0
3	A	10	0	0	0	0
3	B	10	0	0	1	0
3	C	5	0	0	0	0
4	A	43	0	0	0	0
4	B	53	0	0	1	0
4	C	29	0	0	0	0
4	D	60	0	0	0	0
4	E	2	0	0	0	0
4	H	2	0	0	0	0
All	All	12099	0	11956	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (118) 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:84:ARG:HH22	1:B:231:LEU:HG	1.45	0.82
1:C:557:GLU:HG2	1:C:558:GLU:HG2	1.66	0.78
1:B:55:GLU:N	4:B:801:HOH:O	2.23	0.69
1:C:94:VAL:HG22	1:C:109:LYS:HG3	1.79	0.65
1:A:604:LYS:HZ1	2:E:146:ARG:HE	1.45	0.65
1:B:84:ARG:NH2	1:B:231:LEU:HG	2.10	0.65
1:A:227:TYR:HD1	1:A:479:LEU:HD21	1.63	0.64
1:A:76:PHE:HE2	1:A:153:ILE:HD13	1.63	0.63
1:C:215:LYS:C	1:C:540:MET:HE2	2.25	0.62
1:A:213:ASP:OD1	1:A:514:THR:HG23	1.99	0.62
1:D:94:VAL:HG22	1:D:109:LYS:HG2	1.81	0.60
1:D:108:MET:HE3	1:D:151:PHE:HZ	1.68	0.59
1:C:114:ALA:HB3	1:C:117:TYR:HD2	1.67	0.59
1:D:484:GLU:HG3	1:D:486:LYS:HG2	1.84	0.58
1:C:550:LEU:O	2:G:144:ARG:NH2	2.36	0.58
1:B:171:HIS:CE1	1:B:173:LEU:HB3	2.39	0.57
1:B:639:GLU:OE1	1:B:639:GLU:N	2.39	0.56
1:A:227:TYR:CD1	1:A:479:LEU:HD21	2.40	0.56
1:A:521:GLU:OE2	1:A:641:ARG:NH2	2.40	0.55
1:D:104:LYS:NZ	1:D:166:GLU:OE2	2.32	0.55
1:A:633:MET:O	1:A:641:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:LYS:NZ	2:E:146:ARG:HE	2.04	0.54
1:C:168:LEU:HD21	1:C:494:LYS:HD2	1.90	0.54
1:C:68:HIS:HB2	1:C:160:HIS:CD2	2.43	0.54
1:D:114:ALA:HB3	1:D:117:TYR:HD2	1.72	0.54
1:B:227:TYR:O	1:B:231:LEU:HD22	2.08	0.53
1:D:563:GLU:HG3	1:D:590:PHE:HD1	1.74	0.52
1:C:114:ALA:HB3	1:C:117:TYR:CD2	2.45	0.51
1:A:83:ILE:HD11	1:A:98:TRP:HB2	1.94	0.50
1:A:84:ARG:HG2	1:A:85:LYS:N	2.27	0.50
1:B:114:ALA:HB3	1:B:117:TYR:CD2	2.47	0.50
1:D:577:PRO:HG2	1:D:637:ILE:HD11	1.93	0.49
1:D:578:ARG:O	1:D:582:VAL:HG23	2.12	0.49
1:C:557:GLU:H	1:C:557:GLU:CD	2.20	0.49
1:B:226:GLN:HA	1:B:229:ARG:HE	1.77	0.49
1:D:222:SER:OG	1:D:492:LYS:HB2	2.13	0.48
1:A:118:THR:HG23	1:A:161:ILE:HD13	1.96	0.48
1:B:114:ALA:HB3	1:B:117:TYR:HD2	1.78	0.48
1:B:607:GLY:O	1:B:611:VAL:HG23	2.14	0.48
1:C:143:MET:N	1:C:143:MET:SD	2.86	0.48
1:D:484:GLU:CG	1:D:486:LYS:HG2	2.43	0.48
1:A:72:ILE:HD12	1:A:83:ILE:O	2.13	0.48
1:A:635:GLU:O	1:A:641:ARG:NH1	2.42	0.48
1:B:215:LYS:NZ	1:B:514:THR:HG21	2.30	0.47
1:C:172:LEU:O	1:C:176:ILE:HG13	2.14	0.47
1:D:559:TYR:OH	2:F:142:ARG:HG3	2.15	0.47
1:C:68:HIS:HB2	1:C:160:HIS:NE2	2.30	0.47
1:A:194:GLN:HB2	1:A:653:LEU:HD22	1.96	0.46
1:D:172:LEU:O	1:D:176:ILE:HG13	2.16	0.46
1:D:563:GLU:HG3	1:D:590:PHE:CD1	2.51	0.46
1:A:194:GLN:O	1:A:198:GLN:HG3	2.16	0.45
1:C:515:ARG:HD2	1:C:561:ARG:HD2	1.98	0.45
1:C:607:GLY:O	1:C:611:VAL:HG23	2.17	0.45
1:C:609:PHE:HZ	1:C:620:GLN:HG3	1.82	0.45
1:D:579:LYS:H	1:D:579:LYS:NZ	2.14	0.45
1:C:190:LYS:NZ	1:C:655:SER:HA	2.31	0.45
1:D:76:PHE:CB	1:D:108:MET:HE1	2.46	0.45
1:B:68:HIS:HB2	1:B:160:HIS:CD2	2.51	0.45
1:A:588:LYS:HE3	1:D:511:ASP:OD2	2.17	0.45
1:C:190:LYS:HE2	1:C:652:TRP:CE2	2.51	0.45
1:A:215:LYS:NZ	1:A:514:THR:HG21	2.32	0.45
1:B:176:ILE:HD11	1:B:544:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:ASN:HB3	1:B:531:PRO:HD2	1.98	0.45
1:D:114:ALA:HB3	1:D:117:TYR:CD2	2.51	0.45
1:D:567:ALA:O	1:D:571:GLU:HG3	2.17	0.45
1:B:133:ASN:ND2	3:B:702:PO4:O2	2.24	0.44
1:B:190:LYS:HD3	1:B:652:TRP:O	2.17	0.44
1:B:488:ALA:HA	1:B:491:LEU:HD12	1.98	0.44
1:C:194:GLN:HB2	1:C:653:LEU:HD22	1.99	0.44
1:C:626:PHE:CZ	1:C:630:LEU:HD11	2.51	0.44
1:D:517:TYR:OH	1:D:543:GLU:OE1	2.32	0.44
1:B:163:MET:HE2	1:B:165:PHE:CZ	2.52	0.44
1:A:106:VAL:HG13	1:A:164:VAL:HG13	2.00	0.44
2:E:148:ARG:HB3	2:E:149:GLY:H	1.65	0.44
1:D:108:MET:HE3	1:D:151:PHE:CZ	2.50	0.44
1:C:142:GLU:O	1:C:494:LYS:HE2	2.18	0.44
1:D:529:ASN:HB3	1:D:531:PRO:HD2	2.00	0.44
1:C:594:LYS:HE2	1:C:594:LYS:HB2	1.85	0.43
1:B:55:GLU:O	1:B:88:TRP:NE1	2.35	0.43
1:C:224:ASN:O	1:C:228:ILE:HG13	2.18	0.43
1:D:633:MET:O	1:D:641:ARG:HD3	2.18	0.43
1:D:76:PHE:CG	1:D:108:MET:HE1	2.53	0.43
1:C:487:ASN:OD1	1:C:487:ASN:N	2.52	0.43
1:D:127:LEU:O	1:D:131:VAL:HG23	2.18	0.43
1:D:171:HIS:CE1	1:D:173:LEU:HB3	2.54	0.43
1:D:546:THR:HB	1:D:616:TYR:CE1	2.53	0.43
1:A:591:PHE:HA	1:A:596:ASP:O	2.18	0.43
1:C:483:LEU:O	1:C:485:PRO:HD3	2.19	0.43
1:C:227:TYR:CE1	1:C:479:LEU:HD13	2.53	0.42
1:C:230:ARG:C	1:C:232:ALA:H	2.27	0.42
1:D:76:PHE:CD2	1:D:108:MET:HE1	2.53	0.42
1:C:557:GLU:CD	1:C:557:GLU:N	2.78	0.42
1:C:559:TYR:OH	2:G:142:ARG:HG3	2.18	0.42
1:C:214:ILE:HG22	1:C:540:MET:HE3	2.01	0.42
1:A:226:GLN:HA	1:A:229:ARG:HG2	2.02	0.42
1:C:612:LEU:HD22	1:C:618:TRP:CD2	2.55	0.41
1:A:227:TYR:O	1:A:231:LEU:HD13	2.21	0.41
1:D:542:PHE:CG	1:D:550:LEU:HD13	2.55	0.41
1:C:591:PHE:HA	1:C:596:ASP:O	2.20	0.41
1:C:543:GLU:HA	1:C:548:ASP:O	2.21	0.41
1:D:550:LEU:HD23	1:D:551:PHE:CE2	2.55	0.41
1:D:630:LEU:HD23	1:D:630:LEU:HA	1.96	0.41
1:A:70:VAL:HG22	1:A:95:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.85	0.41
1:A:521:GLU:CD	1:A:641:ARG:HH22	2.29	0.41
1:B:84:ARG:HH22	1:B:231:LEU:CG	2.23	0.41
1:C:188:CYS:O	1:C:192:ILE:HG13	2.21	0.41
1:C:512:ILE:O	1:C:513:GLN:HB2	2.20	0.41
1:C:648:LEU:HD23	1:C:648:LEU:HA	1.83	0.41
1:B:94:VAL:HA	1:B:108:MET:O	2.21	0.41
1:C:216:PRO:HG3	1:C:540:MET:HG3	2.03	0.41
1:B:616:TYR:O	1:B:618:TRP:HD1	2.03	0.40
1:A:186:LEU:O	1:A:190:LYS:HG3	2.21	0.40
1:B:68:HIS:HB2	1:B:160:HIS:NE2	2.36	0.40
1:B:171:HIS:CE1	1:B:174:LYS:HG2	2.56	0.40
1:B:193:ILE:HD13	1:B:193:ILE:HA	1.77	0.40
1:A:76:PHE:CD2	1:A:153:ILE:HG21	2.56	0.40
1:B:572:LEU:HD11	1:B:608:LEU:HB2	2.03	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	352/618 (57%)	334 (95%)	18 (5%)	0	100	100
1	B	352/618 (57%)	339 (96%)	10 (3%)	3 (1%)	14	41
1	C	355/618 (57%)	339 (96%)	15 (4%)	1 (0%)	36	66
1	D	352/618 (57%)	336 (96%)	15 (4%)	1 (0%)	36	66
2	E	10/16 (62%)	8 (80%)	2 (20%)	0	100	100
2	F	5/16 (31%)	5 (100%)	0	0	100	100
2	G	6/16 (38%)	5 (83%)	1 (17%)	0	100	100
2	H	6/16 (38%)	5 (83%)	1 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1438/2536 (57%)	1371 (95%)	62 (4%)	5 (0%)	36 66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	232	ALA
1	B	606	TRP
1	B	515	ARG
1	C	515	ARG
1	D	497	ASP

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	315/551 (57%)	304 (96%)	11 (4%)	32 67
1	B	315/551 (57%)	303 (96%)	12 (4%)	29 64
1	C	317/551 (58%)	297 (94%)	20 (6%)	16 45
1	D	315/551 (57%)	298 (95%)	17 (5%)	20 51
2	E	7/8 (88%)	7 (100%)	0	100 100
2	F	5/8 (62%)	4 (80%)	1 (20%)	1 4
2	G	5/8 (62%)	4 (80%)	1 (20%)	1 4
2	H	5/8 (62%)	5 (100%)	0	100 100
All	All	1284/2236 (57%)	1222 (95%)	62 (5%)	23 56

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	106	VAL
1	A	145	VAL
1	A	146	GLN
1	A	168	LEU

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Mol	Chain	Res	Type
1	A	179	SER
1	A	225	GLU
1	A	486	LYS
1	A	530	THR
1	A	588	LYS
1	A	610	GLU
1	B	70	VAL
1	B	86	LEU
1	B	106	VAL
1	B	118	THR
1	B	154	SER
1	B	161	ILE
1	B	166	GLU
1	B	168	LEU
1	B	186	LEU
1	B	223	VAL
1	B	231	LEU
1	B	619	SER
1	C	71	LYS
1	C	84	ARG
1	C	106	VAL
1	C	116	HIS
1	C	168	LEU
1	C	174	LYS
1	C	186	LEU
1	C	223	VAL
1	C	226	GLN
1	C	230	ARG
1	C	478	PHE
1	C	479	LEU
1	C	492	LYS
1	C	514	THR
1	C	524	ILE
1	C	530	THR
1	C	557	GLU
1	C	582	VAL
1	C	601	THR
1	C	619	SER
1	D	106	VAL
1	D	146	GLN
1	D	154	SER
1	D	156	VAL

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Mol	Chain	Res	Type
1	D	161	ILE
1	D	168	LEU
1	D	490	LYS
1	D	498	LEU
1	D	530	THR
1	D	578	ARG
1	D	579	LYS
1	D	580	LEU
1	D	588	LYS
1	D	602	LYS
1	D	610	GLU
1	D	621	GLU
1	D	635	GLU
2	F	142	ARG
2	G	142	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	146	GLN
1	A	198	GLN
1	B	160	HIS
1	B	481	ASN
1	B	513	GLN
1	C	554	HIS
1	D	198	GLN
1	D	513	GLN
1	D	554	HIS
1	D	620	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands 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	$\# Z > 2$
3	PO4	B	701	-	4,4,4	0.91	0	6,6,6	0.76	0
3	PO4	C	701	-	4,4,4	0.74	0	6,6,6	0.94	0
3	PO4	B	702	-	4,4,4	0.78	0	6,6,6	0.65	0
3	PO4	A	701	-	4,4,4	0.83	0	6,6,6	1.08	1 (16%)
3	PO4	A	702	-	4,4,4	1.00	0	6,6,6	0.85	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PO4	O4-P-O3	2.13	114.53	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	356/618 (57%)	-0.06	12 (3%) 48 39	19, 31, 74, 116	0
1	B	356/618 (57%)	0.06	16 (4%) 38 30	21, 35, 77, 142	0
1	C	359/618 (58%)	0.21	17 (4%) 36 29	24, 39, 75, 112	0
1	D	356/618 (57%)	0.05	15 (4%) 40 32	22, 34, 73, 94	0
2	E	12/16 (75%)	0.88	2 (16%) 4 3	31, 52, 67, 73	0
2	F	7/16 (43%)	0.92	1 (14%) 6 5	36, 55, 74, 79	0
2	G	8/16 (50%)	1.15	1 (12%) 8 6	49, 59, 72, 81	0
2	H	8/16 (50%)	1.60	5 (62%) 0 0	39, 67, 86, 87	0
All	All	1462/2536 (57%)	0.09	69 (4%) 36 29	19, 36, 75, 142	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	TYR	6.4
1	B	233	ALA	6.3
1	C	478	PHE	5.5
1	A	233	ALA	5.4
1	B	232	ALA	5.4
1	B	224	ASN	5.3
1	A	232	ALA	4.8
1	D	232	ALA	4.1
1	B	231	LEU	4.1
1	C	232	ALA	4.0
1	D	233	ALA	3.9
1	C	233	ALA	3.6
1	C	557	GLU	3.6
1	A	224	ASN	3.5
1	D	91	PHE	3.4
1	D	90	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	149	GLY	3.3
1	A	479	LEU	3.2
1	A	227	TYR	3.1
1	D	594	LYS	3.1
1	B	480	VAL	3.1
1	C	486	LYS	3.0
1	B	655	SER	2.9
2	G	145	ARG	2.9
1	A	231	LEU	2.9
1	B	226	GLN	2.8
1	D	224	ASN	2.8
1	A	225	GLU	2.8
1	C	231	LEU	2.7
2	H	149	GLY	2.7
1	A	226	GLN	2.7
1	A	655	SER	2.7
1	D	226	GLN	2.7
2	H	146	ARG	2.7
1	D	558	GLU	2.6
1	B	230	ARG	2.6
1	C	477	ASN	2.6
1	C	575	LYS	2.6
1	B	170	HIS	2.5
1	C	55	GLU	2.5
1	C	588	LYS	2.5
2	H	147	GLY	2.4
1	A	602	LYS	2.3
2	H	145	ARG	2.3
1	D	60	ASN	2.3
1	C	230	ARG	2.3
1	B	622	GLU	2.3
1	D	231	LEU	2.3
1	D	116	HIS	2.3
1	C	655	SER	2.3
1	C	476	GLY	2.2
1	B	484	GLU	2.2
1	B	479	LEU	2.2
1	D	227	TYR	2.2
1	C	479	LEU	2.2
1	C	593	LYS	2.2
2	E	138	ARG	2.1
1	B	225	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	589	GLU	2.1
1	A	228	ILE	2.1
1	D	88	TRP	2.1
1	B	228	ILE	2.1
1	D	230	ARG	2.1
1	A	116	HIS	2.1
2	F	148	ARG	2.1
1	D	621	GLU	2.1
1	B	602	LYS	2.0
2	H	148	ARG	2.0
1	C	602	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	B	702	5/5	0.83	0.22	40,53,62,68	0
3	PO4	C	701	5/5	0.92	0.20	24,42,55,56	0
3	PO4	A	701	5/5	0.94	0.10	31,31,55,66	0
3	PO4	B	701	5/5	0.94	0.12	51,52,54,59	0
3	PO4	A	702	5/5	0.96	0.12	37,43,47,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.