



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:04 AM UTC

PDB ID : 6SWU / pdb_00006swu
Title : Crystal structure of the TPR domain of KLC1 in complex with an engineered high-affinity cargo peptide.
Authors : Chegkazi, M.S.; Steiner, R.A.
Deposited on : 2019-09-23
Resolution : 2.85 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

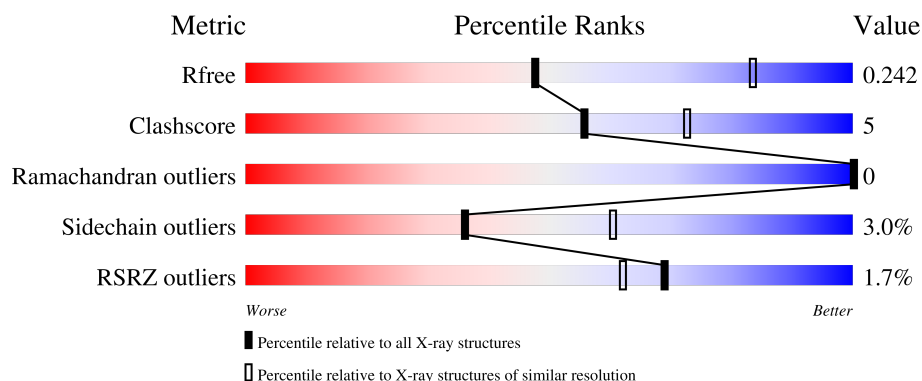
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	343	72% 13% 14%
1	B	343	74% 8% 16%
1	C	343	3% 72% 11% 16%
1	D	343	2% 72% 10% 16%
1	E	343	72% 8% 18%

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Mol	Chain	Length	Quality of chain
1	F	343	% 72% 9% • 18%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27765 atoms, of which 13832 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 Kinesin light chain 1, Kinesin light chain 1, TPR domain of kinesin light chain 1 in complex with an engineered high-affinity cargo peptide of sequence TVFTTEDIYEWDDSAI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	H	N	O	S	117	0	0
			4709	1479	2352	418	451	9			
1	B	288	Total	C	H	N	O	S	113	1	0
			4639	1456	2322	412	440	9			
1	C	287	Total	C	H	N	O	S	114	0	0
			4588	1446	2289	404	440	9			
1	D	287	Total	C	H	N	O	S	114	0	0
			4602	1449	2297	407	440	9			
1	E	281	Total	C	H	N	O	S	112	0	0
			4501	1416	2246	400	431	8			
1	F	281	Total	C	H	N	O	S	112	0	0
			4510	1419	2252	400	431	8			

There are 24 discrepancies between the modelled and reference sequences:

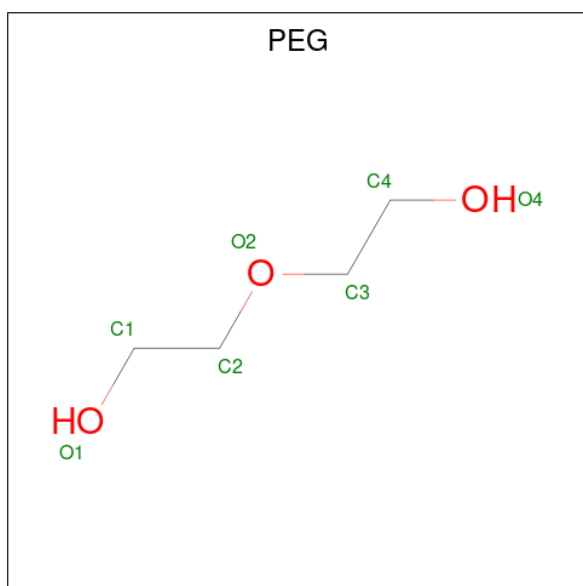
Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLY	-	expression tag	UNP Q5UE59
A	202	SER	-	expression tag	UNP Q5UE59
A	203	HIS	-	expression tag	UNP Q5UE59
A	204	MET	-	expression tag	UNP Q5UE59
B	201	GLY	-	expression tag	UNP Q5UE59
B	202	SER	-	expression tag	UNP Q5UE59
B	203	HIS	-	expression tag	UNP Q5UE59
B	204	MET	-	expression tag	UNP Q5UE59
C	201	GLY	-	expression tag	UNP Q5UE59
C	202	SER	-	expression tag	UNP Q5UE59
C	203	HIS	-	expression tag	UNP Q5UE59
C	204	MET	-	expression tag	UNP Q5UE59
D	201	GLY	-	expression tag	UNP Q5UE59
D	202	SER	-	expression tag	UNP Q5UE59
D	203	HIS	-	expression tag	UNP Q5UE59

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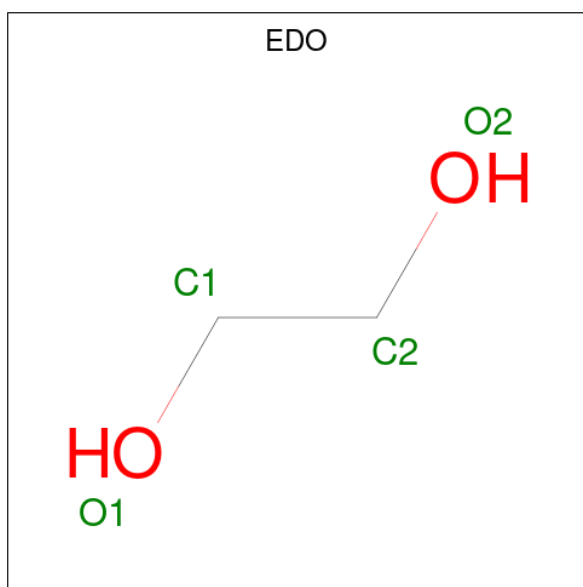
Chain	Residue	Modelled	Actual	Comment	Reference
D	204	MET	-	expression tag	UNP Q5UE59
E	201	GLY	-	expression tag	UNP Q5UE59
E	202	SER	-	expression tag	UNP Q5UE59
E	203	HIS	-	expression tag	UNP Q5UE59
E	204	MET	-	expression tag	UNP Q5UE59
F	201	GLY	-	expression tag	UNP Q5UE59
F	202	SER	-	expression tag	UNP Q5UE59
F	203	HIS	-	expression tag	UNP Q5UE59
F	204	MET	-	expression tag	UNP Q5UE59

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	1	0
			17	4	10	3		
2	A	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	1	0
			10	2	6	2		
3	C	1	Total	C	H	O	1	0
			10	2	6	2		
3	C	1	Total	C	H	O	1	0
			10	2	6	2		
3	C	1	Total	C	H	O	1	0
			10	2	6	2		
3	D	1	Total	C	H	O	1	0
			10	2	6	2		
3	D	1	Total	C	H	O	1	0
			10	2	6	2		
3	D	1	Total	C	H	O	1	0
			10	2	6	2		
3	E	1	Total	C	H	O	1	0
			10	2	6	2		
3	F	1	Total	C	H	O	1	0
			10	2	6	2		

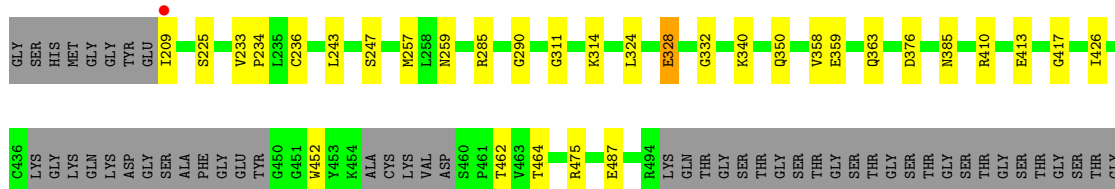
- Molecule 4 is water.

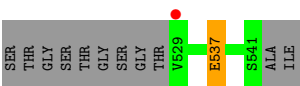
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	19	Total	O	0	0
			19	19		
4	C	18	Total	O	0	0
			18	18		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	13	Total 13	O 13	0	0
4	E	3	Total 3	O 3	0	0
4	F	13	Total 13	O 13	0	0





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.73Å 107.53Å 222.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.33 – 2.85 111.33 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (111.33-2.85) 99.2 (111.33-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.202 , 0.243 0.202 , 0.242	Depositor DCC
R_{free} test set	2704 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27765	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

5.1 Standard geometry

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

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	0.96	0/2398	1.55	8/3233 (0.2%)
1	B	0.99	0/2359	1.50	6/3180 (0.2%)
1	C	0.98	0/2340	1.50	3/3160 (0.1%)
1	D	0.96	0/2346	1.50	6/3167 (0.2%)
1	E	0.96	0/2294	1.49	6/3094 (0.2%)
1	F	0.94	0/2297	1.48	2/3099 (0.1%)
All	All	0.97	0/14034	1.50	31/18933 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	2
1	F	0	1
All	All	0	4

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	332	GLY	CA-C-O	-8.05	116.16	122.52
1	C	332	GLY	CA-C-O	-6.64	117.65	122.23
1	D	312	LYS	CA-C-O	-6.57	112.80	120.62
1	D	332	GLY	CA-C-O	-6.34	117.86	122.23
1	E	290	GLY	CA-C-N	6.23	129.25	120.28
1	E	290	GLY	C-N-CA	6.23	129.25	120.28
1	A	415	GLU	CB-CG-CD	6.18	123.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	GLY	CA-C-O	-6.15	117.98	122.23
1	C	542	ALA	CA-C-O	6.14	131.23	120.80
1	A	248	GLY	CA-C-O	-6.00	116.13	121.41
1	D	475	ARG	CG-CD-NE	-5.84	99.15	112.00
1	F	290	GLY	CA-C-O	-5.72	118.28	122.23
1	D	290	GLY	CA-C-O	-5.72	118.29	122.23
1	E	540	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	459	ASP	CA-C-N	5.61	128.64	120.51
1	A	459	ASP	C-N-CA	5.61	128.64	120.51
1	B	290	GLY	CA-C-O	-5.57	117.53	121.88
1	B	399	GLN	CB-CG-CD	-5.52	103.21	112.60
1	B	209	ILE	N-CA-CB	5.42	113.91	110.50
1	D	460	SER	CA-C-N	5.36	124.87	119.19
1	D	460	SER	C-N-CA	5.36	124.87	119.19
1	F	332	GLY	CA-C-O	-5.35	118.54	122.23
1	A	290	GLY	CA-C-O	-5.35	118.54	122.23
1	B	291	ARG	CA-C-O	-5.32	115.76	121.56
1	C	290	GLY	CA-C-O	-5.31	118.57	122.23
1	A	249	HIS	CA-C-O	-5.25	115.84	121.56
1	A	332	GLY	CA-C-O	-5.22	118.63	122.23
1	E	290	GLY	CA-C-O	-5.19	118.65	122.23
1	A	441	LYS	CA-C-O	-5.07	115.04	120.46
1	B	292	ASP	CA-CB-CG	5.03	117.63	112.60
1	E	210	PRO	N-CA-CB	5.03	108.53	103.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	312	LYS	Mainchain
1	E	311	GLY	Peptide
1	E	332	GLY	Mainchain
1	F	311	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2357	2352	2343	28	0
1	B	2317	2322	2312	17	0
1	C	2299	2289	2279	24	0
1	D	2305	2297	2287	21	0
1	E	2255	2246	2236	24	0
1	F	2258	2252	2241	22	0
2	A	14	20	20	0	0
3	C	16	24	24	0	0
3	D	12	18	18	0	0
3	E	4	6	6	0	0
3	F	4	6	6	0	0
4	A	26	0	0	0	0
4	B	19	0	0	1	0
4	C	18	0	0	0	0
4	D	13	0	0	0	0
4	E	3	0	0	0	0
4	F	13	0	0	0	0
All	All	13933	13832	13772	131	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 (131) 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:236:CYS:SG	1:B:257:MET:HE1	1.89	1.11
1:E:412:HIS:HE1	1:E:423:ASN:OD1	1.35	1.09
1:E:412:HIS:CE1	1:E:423:ASN:OD1	2.13	1.00
1:B:236:CYS:SG	1:B:257:MET:CE	2.50	0.99
1:D:313:TYR:OH	1:D:351:ASN:ND2	1.96	0.97
1:C:236:CYS:SG	1:C:257:MET:HE1	2.05	0.94
1:C:236:CYS:SG	1:C:257:MET:CE	2.56	0.93
1:D:236:CYS:SG	1:D:257:MET:HE1	2.08	0.93
1:F:236:CYS:SG	1:F:257:MET:HE1	2.09	0.91
1:D:313:TYR:CZ	1:D:351:ASN:ND2	2.38	0.90
1:E:236:CYS:SG	1:E:257:MET:HE1	2.12	0.90
1:A:454:LYS:O	1:A:458:VAL:HG12	1.72	0.89
1:E:236:CYS:SG	1:E:257:MET:CE	2.61	0.89
1:D:236:CYS:SG	1:D:257:MET:CE	2.61	0.89
1:E:330:VAL:HG13	1:E:331:LEU:HD22	1.55	0.88
1:F:236:CYS:SG	1:F:257:MET:CE	2.61	0.87
1:E:298:ALA:CB	1:E:539:ASP:OD2	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:ALA:HA	1:E:539:ASP:OD2	1.84	0.78
1:E:421:ASP:O	1:E:424:LYS:CE	2.32	0.76
1:E:298:ALA:HB2	1:E:539:ASP:OD2	1.87	0.74
1:B:347:LEU:HD12	1:B:362:TYR:OH	1.90	0.72
1:B:359:GLU:O	1:B:363:GLN:HG2	1.89	0.72
1:C:376:ASP:HB3	1:C:414:ARG:HD3	1.69	0.72
1:E:421:ASP:O	1:E:424:LYS:HE2	1.88	0.72
1:A:236:CYS:SG	1:A:257:MET:CE	2.79	0.71
1:D:359:GLU:O	1:D:363:GLN:HG2	1.90	0.70
1:E:298:ALA:CA	1:E:539:ASP:OD2	2.39	0.70
1:D:535:ILE:HG13	1:D:535:ILE:O	1.93	0.69
1:A:236:CYS:SG	1:A:257:MET:HE3	2.33	0.69
1:D:393:LYS:HE3	1:D:532:THR:HG21	1.78	0.65
1:B:251:HIS:HD2	1:B:253:ASP:H	1.44	0.65
1:E:421:ASP:O	1:E:424:LYS:HE3	1.95	0.65
1:A:366:LEU:O	1:A:370:GLN:HG3	1.98	0.64
1:F:324:LEU:O	1:F:328:GLU:HG2	1.97	0.64
1:A:366:LEU:HG	1:A:370:GLN:HE21	1.64	0.62
1:A:436:CYS:HB3	1:A:439:LYS:HB3	1.80	0.62
1:E:330:VAL:HG13	1:E:331:LEU:CD2	2.29	0.62
1:C:385:ASN:HD21	1:C:466:THR:HG23	1.64	0.62
1:B:236:CYS:SG	1:B:257:MET:HE3	2.40	0.62
1:C:385:ASN:HD21	1:C:466:THR:CG2	2.13	0.61
1:F:340:LYS:HE3	1:F:537:GLU:CG	2.31	0.61
1:E:314:LYS:HE3	1:E:352:GLN:OE1	2.00	0.61
1:E:210:PRO:HD2	1:E:213:LEU:HD12	1.84	0.60
1:F:385:ASN:HD22	1:F:462:THR:HG22	1.66	0.60
1:A:440:GLN:HA	1:A:440:GLN:OE1	2.01	0.60
1:F:385:ASN:HD22	1:F:462:THR:CG2	2.14	0.60
1:F:259:ASN:HD21	1:F:285:ARG:NH1	2.00	0.59
1:F:340:LYS:HE3	1:F:537:GLU:HG2	1.84	0.59
1:C:236:CYS:SG	1:C:257:MET:HE3	2.41	0.58
1:C:460:SER:HB3	1:C:463:VAL:HB	1.85	0.58
1:A:385:ASN:HD21	1:A:466:THR:HG23	1.69	0.58
1:F:236:CYS:SG	1:F:257:MET:HE3	2.44	0.58
1:E:236:CYS:SG	1:E:257:MET:HE3	2.44	0.57
1:A:236:CYS:SG	1:A:257:MET:HE1	2.43	0.57
1:E:321:LYS:O	1:E:325:GLU:HG3	2.06	0.55
1:F:359:GLU:O	1:F:363:GLN:HG3	2.05	0.55
1:A:228:ARG:HH22	1:F:234:PRO:HG3	1.72	0.55
1:C:529:VAL:HG12	1:C:529:VAL:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:LEU:HD13	1:D:426:ILE:CD1	2.38	0.54
1:D:236:CYS:SG	1:D:257:MET:HE3	2.47	0.54
1:D:532:THR:HG22	1:D:532:THR:O	2.08	0.53
1:C:340:LYS:HE3	1:C:537:GLU:CG	2.37	0.53
1:A:532:THR:HG22	1:A:532:THR:O	2.08	0.52
1:E:418:SER:O	1:E:423:ASN:ND2	2.42	0.52
1:F:233:VAL:HB	1:F:234:PRO:HD3	1.92	0.51
1:B:251:HIS:CD2	1:B:253:ASP:H	2.26	0.51
1:B:291:ARG:HB2	1:B:322[A]:ARG:HH21	1.75	0.51
1:C:532:THR:O	1:C:532:THR:HG22	2.10	0.51
1:C:340:LYS:HE3	1:C:537:GLU:HG2	1.92	0.51
1:F:259:ASN:ND2	1:F:285:ARG:NH1	2.57	0.51
1:A:382:LYS:HG2	1:A:462:THR:HG21	1.93	0.51
1:F:475:ARG:NH1	1:F:487:GLU:OE2	2.36	0.51
1:A:233:VAL:HB	1:A:234:PRO:HD3	1.93	0.50
1:B:532:THR:O	1:B:532:THR:HG22	2.12	0.48
1:E:538:TRP:HD1	1:E:540:ASP:HB3	1.79	0.48
1:D:464:THR:HG22	1:D:493:SER:OG	2.14	0.47
1:F:385:ASN:ND2	1:F:462:THR:HG22	2.30	0.47
1:A:455:ALA:O	1:A:459:ASP:CG	2.58	0.47
1:B:359:GLU:O	1:B:363:GLN:CG	2.60	0.46
1:D:233:VAL:HB	1:D:234:PRO:HD3	1.97	0.46
1:C:233:VAL:HB	1:C:234:PRO:HD3	1.98	0.46
1:A:242:ASP:O	1:A:246:THR:HG23	2.15	0.46
1:A:252:PRO:O	1:A:256:THR:HG23	2.15	0.46
1:A:458:VAL:HG22	1:A:458:VAL:O	2.16	0.46
1:C:475:ARG:NH1	1:C:487:GLU:OE1	2.46	0.45
1:E:233:VAL:HB	1:E:234:PRO:HD3	1.97	0.45
1:B:233:VAL:HB	1:B:234:PRO:HD3	1.99	0.45
1:B:292:ASP:HA	1:B:326:ILE:HG12	1.99	0.45
1:B:464:THR:HG22	1:B:493:SER:OG	2.17	0.45
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.84	0.44
1:C:259:ASN:ND2	1:C:285:ARG:NH1	2.65	0.44
1:C:462:THR:O	1:C:466:THR:HG23	2.18	0.44
1:D:458:VAL:HG22	1:D:458:VAL:O	2.17	0.44
1:A:350:GLN:HA	1:A:358:VAL:HG21	2.00	0.43
1:A:454:LYS:C	1:A:458:VAL:HG12	2.40	0.43
1:A:266:ARG:HD3	1:A:538:TRP:CH2	2.54	0.43
1:A:250:ASP:HA	1:A:284:ILE:HG12	2.00	0.43
1:C:350:GLN:HA	1:C:358:VAL:HG21	2.00	0.43
1:A:359:GLU:O	1:A:363:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:ASP:OD1	1:F:410:ARG:NH1	2.50	0.43
1:A:490:ALA:O	1:A:494:ARG:HG3	2.19	0.43
1:C:376:ASP:CB	1:C:414:ARG:HD3	2.43	0.43
1:C:317:GLU:OE1	1:C:354:LYS:NZ	2.51	0.42
1:C:413:GLU:HA	1:C:417:GLY:O	2.19	0.42
1:C:366:LEU:HD12	1:C:366:LEU:HA	1.90	0.42
1:F:350:GLN:HA	1:F:358:VAL:HG21	2.01	0.42
1:F:376:ASP:OD1	1:F:410:ARG:NE	2.52	0.42
1:E:475:ARG:NH1	1:E:487:GLU:OE1	2.46	0.42
1:D:350:GLN:HA	1:D:358:VAL:HG21	2.01	0.42
1:A:228:ARG:NH2	1:F:234:PRO:HG3	2.33	0.42
1:D:213:LEU:HD13	1:D:243:LEU:HD13	2.01	0.42
1:F:413:GLU:HA	1:F:417:GLY:O	2.20	0.42
1:C:407:ILE:HG21	1:C:466:THR:HG21	2.01	0.41
1:B:259:ASN:ND2	1:B:542:ALA:HB1	2.36	0.41
1:C:376:ASP:OD1	1:C:410:ARG:HD2	2.20	0.41
1:E:535:ILE:O	1:E:535:ILE:HG13	2.20	0.41
1:C:492:ARG:NH2	1:D:541:SER:HA	2.35	0.41
1:A:317:GLU:OE1	1:A:354:LYS:NZ	2.51	0.41
1:E:413:GLU:HA	1:E:417:GLY:O	2.20	0.41
1:E:539:ASP:HA	1:F:452:TRP:NE1	2.36	0.41
1:D:272:LYS:HE3	1:D:310:ARG:HH12	1.85	0.41
1:D:413:GLU:HA	1:D:417:GLY:O	2.21	0.41
1:B:212:ARG:NH1	4:B:601:HOH:O	2.42	0.41
1:D:317:GLU:OE1	1:D:354:LYS:NZ	2.53	0.41
1:A:452:TRP:HB3	1:B:337:ASP:CG	2.45	0.41
1:F:340:LYS:HE3	1:F:537:GLU:HG3	1.99	0.41
1:C:251:HIS:HD2	1:C:253:ASP:HB2	1.84	0.41
1:D:366:LEU:HG	1:D:370:GLN:NE2	2.36	0.41
1:A:455:ALA:O	1:A:459:ASP:CB	2.69	0.40
1:B:413:GLU:HA	1:B:417:GLY:O	2.20	0.40
1:D:213:LEU:HD23	1:D:213:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

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	288/343 (84%)	286 (99%)	2 (1%)	0	100	100
1	B	281/343 (82%)	277 (99%)	4 (1%)	0	100	100
1	C	281/343 (82%)	279 (99%)	2 (1%)	0	100	100
1	D	281/343 (82%)	278 (99%)	3 (1%)	0	100	100
1	E	273/343 (80%)	270 (99%)	3 (1%)	0	100	100
1	F	273/343 (80%)	271 (99%)	2 (1%)	0	100	100
All	All	1677/2058 (82%)	1661 (99%)	16 (1%)	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	247/279 (88%)	242 (98%)	5 (2%)	48	72
1	B	243/279 (87%)	235 (97%)	8 (3%)	33	58
1	C	241/279 (86%)	234 (97%)	7 (3%)	37	61
1	D	242/279 (87%)	232 (96%)	10 (4%)	27	52
1	E	236/279 (85%)	231 (98%)	5 (2%)	47	70
1	F	237/279 (85%)	228 (96%)	9 (4%)	29	54
All	All	1446/1674 (86%)	1402 (97%)	44 (3%)	36	60

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	SER
1	A	263	LEU
1	A	347	LEU

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Mol	Chain	Res	Type
1	A	435	GLU
1	A	529	VAL
1	B	247	SER
1	B	259	ASN
1	B	370	GLN
1	B	372	LYS
1	B	398	LYS
1	B	426	ILE
1	B	437	LYS
1	B	464	THR
1	C	225	SER
1	C	247	SER
1	C	263	LEU
1	C	325	GLU
1	C	363	GLN
1	C	464	THR
1	C	537	GLU
1	D	225	SER
1	D	241	GLU
1	D	243	LEU
1	D	259	ASN
1	D	263	LEU
1	D	422	GLU
1	D	426	ILE
1	D	464	THR
1	D	492	ARG
1	D	541	SER
1	E	225	SER
1	E	263	LEU
1	E	462	THR
1	E	464	THR
1	E	535	ILE
1	F	209	ILE
1	F	225	SER
1	F	243	LEU
1	F	247	SER
1	F	314	LYS
1	F	328	GLU
1	F	426	ILE
1	F	464	THR
1	F	537	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	238	GLN
1	A	343	ASN
1	A	363	GLN
1	A	370	GLN
1	A	379	ASN
1	A	385	ASN
1	A	386	ASN
1	A	394	GLN
1	A	429	HIS
1	B	238	GLN
1	B	251	HIS
1	B	343	ASN
1	B	370	GLN
1	B	386	ASN
1	B	429	HIS
1	C	238	GLN
1	C	249	HIS
1	C	251	HIS
1	C	259	ASN
1	C	276	ASN
1	C	343	ASN
1	C	385	ASN
1	C	386	ASN
1	C	394	GLN
1	C	429	HIS
1	D	226	GLN
1	D	343	ASN
1	D	351	ASN
1	D	363	GLN
1	D	370	GLN
1	D	386	ASN
1	D	399	GLN
1	D	429	HIS
1	E	249	HIS
1	E	343	ASN
1	E	351	ASN
1	E	386	ASN
1	E	412	HIS
1	F	222	GLN
1	F	259	ASN
1	F	276	ASN

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Mol	Chain	Res	Type
1	F	343	ASN
1	F	385	ASN
1	F	386	ASN
1	F	399	GLN
1	F	429	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	EDO	C	604	-	3,3,3	0.17	0	2,2,2	0.34	0
3	EDO	D	601	-	3,3,3	0.09	0	2,2,2	0.16	0
3	EDO	E	601	-	3,3,3	0.09	0	2,2,2	0.15	0
2	PEG	A	601	-	6,6,6	0.18	0	5,5,5	0.08	0
3	EDO	C	601	-	3,3,3	0.13	0	2,2,2	0.25	0
3	EDO	D	603	-	3,3,3	0.11	0	2,2,2	0.19	0
3	EDO	F	601	-	3,3,3	0.18	0	2,2,2	0.25	0
3	EDO	D	602	-	3,3,3	0.07	0	2,2,2	0.11	0
2	PEG	A	602	-	6,6,6	0.24	0	5,5,5	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	603	-	3,3,3	0.11	0	2,2,2	0.11	0
3	EDO	C	602	-	3,3,3	0.16	0	2,2,2	0.25	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	EDO	C	604	-	-	0/1/1/1	-
3	EDO	D	601	-	-	0/1/1/1	-
3	EDO	E	601	-	-	0/1/1/1	-
2	PEG	A	601	-	-	3/4/4/4	-
3	EDO	C	601	-	-	0/1/1/1	-
3	EDO	D	603	-	-	0/1/1/1	-
3	EDO	F	601	-	-	0/1/1/1	-
3	EDO	D	602	-	-	1/1/1/1	-
2	PEG	A	602	-	-	4/4/4/4	-
3	EDO	C	603	-	-	1/1/1/1	-
3	EDO	C	602	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	PEG	O2-C3-C4-O4
2	A	601	PEG	O1-C1-C2-O2
2	A	601	PEG	O2-C3-C4-O4
3	C	603	EDO	O1-C1-C2-O2
2	A	602	PEG	O1-C1-C2-O2
3	D	602	EDO	O1-C1-C2-O2
2	A	601	PEG	C1-C2-O2-C3
2	A	602	PEG	C4-C3-O2-C2
2	A	602	PEG	C1-C2-O2-C3

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	294/343 (85%)	-0.25	4 (1%) 73 67	43, 71, 127, 161	0
1	B	288/343 (83%)	-0.33	3 (1%) 79 75	34, 67, 110, 155	1 (0%)
1	C	287/343 (83%)	-0.23	9 (3%) 51 42	40, 70, 118, 159	0
1	D	287/343 (83%)	0.03	7 (2%) 59 50	55, 92, 130, 162	0
1	E	281/343 (81%)	0.09	4 (1%) 73 67	66, 116, 151, 171	0
1	F	281/343 (81%)	-0.17	2 (0%) 84 80	55, 89, 134, 154	0
All	All	1718/2058 (83%)	-0.14	29 (1%) 69 62	34, 84, 137, 171	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	542	ALA	3.9
1	F	209	ILE	3.7
1	A	542	ALA	3.6
1	A	458	VAL	3.4
1	E	529	VAL	3.0
1	C	529	VAL	3.0
1	F	529	VAL	3.0
1	D	449	TYR	2.9
1	C	436	CYS	2.8
1	D	458	VAL	2.7
1	A	449	TYR	2.7
1	C	435	GLU	2.7
1	B	457	LYS	2.6
1	D	436	CYS	2.6
1	C	531	THR	2.5
1	B	529	VAL	2.5
1	E	455	ALA	2.5
1	C	209	ILE	2.4
1	D	209	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	531	THR	2.4
1	C	457	LYS	2.3
1	D	360	TYR	2.3
1	B	543	ILE	2.3
1	C	532	THR	2.2
1	C	449	TYR	2.2
1	A	442	ASP	2.2
1	D	246	THR	2.1
1	E	541	SER	2.1
1	D	529	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 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	EDO	E	601	4/4	0.60	0.21	106,109,110,111	1
3	EDO	D	602	4/4	0.67	0.17	105,107,108,110	1
3	EDO	C	602	4/4	0.69	0.20	90,97,100,110	1
3	EDO	D	601	4/4	0.73	0.20	104,106,108,110	1
3	EDO	C	603	4/4	0.81	0.15	87,95,98,110	1
3	EDO	F	601	4/4	0.82	0.21	93,98,103,110	1
3	EDO	D	603	4/4	0.85	0.14	91,103,104,110	1
2	PEG	A	602	7/7	0.87	0.17	99,102,105,110	1
3	EDO	C	601	4/4	0.88	0.15	87,90,93,110	1
3	EDO	C	604	4/4	0.89	0.19	93,102,105,110	1
2	PEG	A	601	7/7	0.94	0.12	94,103,110,113	1

6.5 Other polymers [i](#)

There are no such residues in this entry.