



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:08 PM UTC

PDB ID : 6Q5Y / pdb_00006q5y
Title : Crystal structure of the SPOC domain of human PHF3 in complex with RNA polymerase II CTD diheptapeptide phosphorylated on Ser2Ser5
Authors : Grishkovskaya, I.; Djinovic-Carugo, K.; Slade, D.
Deposited on : 2018-12-09
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

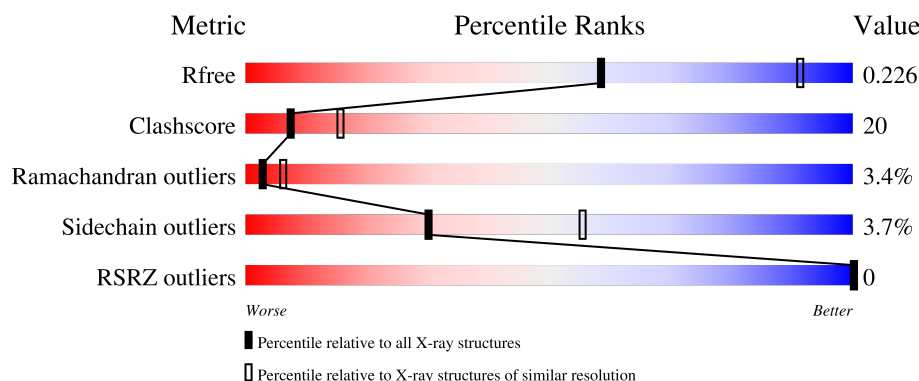
1 Overall quality at a glance

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.



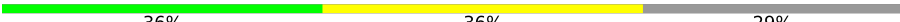
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	162	
1	B	162	
1	C	162	
1	D	162	
2	E	14	

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Mol	Chain	Length	Quality of chain
2	F	14	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (36%), yellow (36%), and grey (29%).

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4918 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 PHD finger protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1190	775	199	212	4			
1	B	148	Total	C	N	O	S	4	0	0
			1181	769	197	211	4			
1	C	148	Total	C	N	O	S	0	0	0
			1181	770	197	210	4			
1	D	149	Total	C	N	O	S	4	0	0
			1190	775	199	212	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1195	GLY	-	expression tag	UNP Q92576
A	1196	ALA	-	expression tag	UNP Q92576
A	1197	MET	-	expression tag	UNP Q92576
A	1198	GLY	-	expression tag	UNP Q92576
B	1195	GLY	-	expression tag	UNP Q92576
B	1196	ALA	-	expression tag	UNP Q92576
B	1197	MET	-	expression tag	UNP Q92576
B	1198	GLY	-	expression tag	UNP Q92576
C	1195	GLY	-	expression tag	UNP Q92576
C	1196	ALA	-	expression tag	UNP Q92576
C	1197	MET	-	expression tag	UNP Q92576
C	1198	GLY	-	expression tag	UNP Q92576
D	1195	GLY	-	expression tag	UNP Q92576
D	1196	ALA	-	expression tag	UNP Q92576
D	1197	MET	-	expression tag	UNP Q92576
D	1198	GLY	-	expression tag	UNP Q92576

- Molecule 2 is a protein called pSer2pSer5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	10	Total 83	C 44	N 10	O 26	P 3	0	0	0
2	F	10	Total 83	C 44	N 10	O 26	P 3	0	0	0

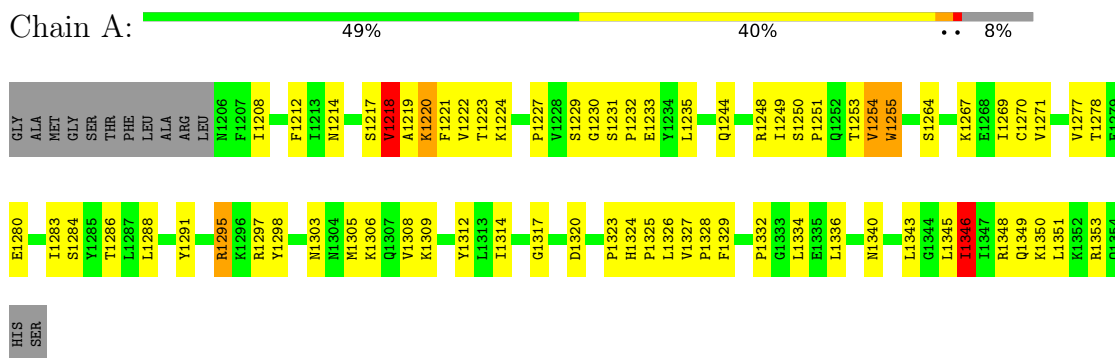
- Molecule 3 is water.

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

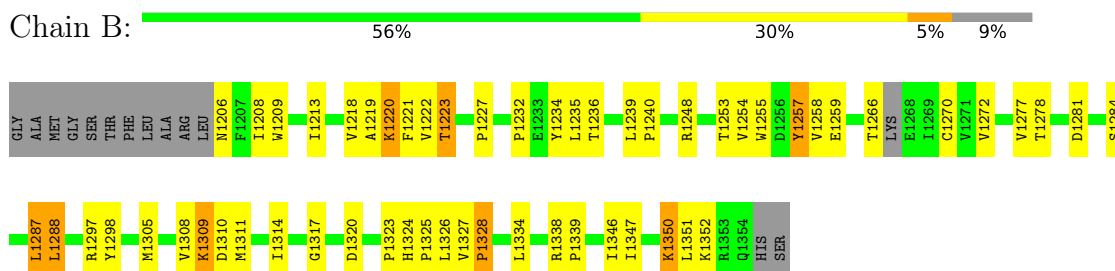
3 Residue-property plots

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.

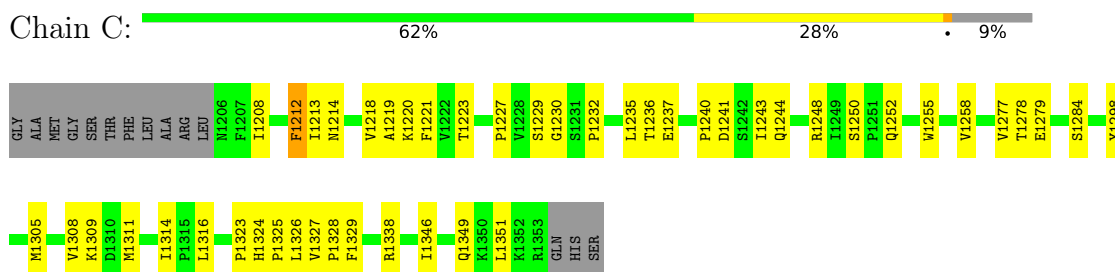
- Molecule 1: PHD finger protein 3



- Molecule 1: PHD finger protein 3



- Molecule 1: PHD finger protein 3

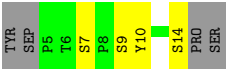


- Molecule 1: PHD finger protein 3

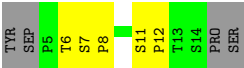
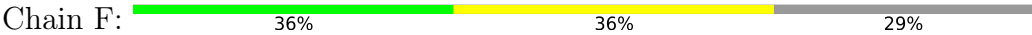




• Molecule 2: pSer2pSer5



• Molecule 2: pSer2pSer5



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	67.83Å 67.83Å 178.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.76 – 2.85 41.76 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.76-2.85) 98.8 (41.76-2.85)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.192 , 0.227 0.193 , 0.226	Depositor DCC
R_{free} test set	1018 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.428 for -h,-k,l 0.438 for h,-h-k,-l 0.427 for -k,-h,-l	Xtriage
Reported twinning fraction	0.262 for H, K, L 0.233 for K, H, -L 0.251 for -K, -H, -L 0.254 for -h,-k,l	Depositor
Outliers	0 of 21141 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4918	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% 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: SEP

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	1.04	0/1221	1.41	3/1657 (0.2%)
1	B	1.22	1/1211 (0.1%)	1.37	2/1643 (0.1%)
1	C	1.01	0/1212	1.33	1/1645 (0.1%)
1	D	1.01	0/1221	1.34	2/1657 (0.1%)
2	E	0.67	0/54	1.16	0/70
2	F	0.69	0/54	1.17	0/70
All	All	1.07	1/4973 (0.0%)	1.36	8/6742 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1220	LYS	CB-CG	-22.01	0.86	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1220	LYS	CA-CB-CG	5.87	125.83	114.10
1	B	1257	TYR	CB-CA-C	5.77	118.38	109.03
1	A	1320	ASP	CA-C-O	-5.68	115.04	121.00
1	D	1305	MET	CA-C-N	5.36	128.86	120.82
1	D	1305	MET	C-N-CA	5.36	128.86	120.82
1	C	1230	GLY	CA-C-O	-5.28	118.52	122.37
1	A	1255	TRP	CA-C-N	5.18	127.73	120.28
1	A	1255	TRP	C-N-CA	5.18	127.73	120.28

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	1190	0	1219	76	1
1	B	1181	0	1205	39	1
1	C	1181	0	1211	36	0
1	D	1190	0	1219	56	0
2	E	83	0	60	4	0
2	F	83	0	60	4	0
3	A	3	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	4	0	0	0	0
3	E	1	0	0	0	0
All	All	4918	0	4974	201	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (201) 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:1317:GLY:O	1:B:1338:ARG:NH1	1.62	1.32
1:C:1349:GLN:HE22	1:C:1351:LEU:HB2	1.13	1.11
1:A:1305:MET:HB3	1:A:1308:VAL:O	1.54	1.07
1:C:1241:ASP:OD2	1:D:1214:ASN:ND2	1.97	0.97
1:A:1229:SER:HB3	1:A:1271:VAL:HG12	1.43	0.97
1:C:1248:ARG:NH1	2:E:14:SEP:O1P	2.08	0.86
1:C:1349:GLN:HE22	1:C:1351:LEU:CB	1.90	0.85
1:A:1291:TYR:O	1:A:1295:ARG:HG2	1.77	0.84
1:C:1349:GLN:NE2	1:C:1351:LEU:HB2	1.93	0.84
1:A:1229:SER:HB3	1:A:1271:VAL:CG1	2.13	0.78
1:A:1253:THR:HG21	2:E:9:SER:HB2	1.65	0.77
1:B:1327:VAL:HG23	1:B:1328:PRO:HD3	1.67	0.77
1:B:1309:LYS:HB2	1:B:1347:ILE:O	1.86	0.76
1:A:1327:VAL:HG23	1:A:1328:PRO:HD3	1.66	0.76
1:A:1295:ARG:O	1:A:1297:ARG:NE	2.19	0.75
1:A:1305:MET:HB3	1:A:1308:VAL:HG13	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1324:HIS:O	1:A:1327:VAL:HG22	1.86	0.74
1:D:1238:ASP:O	1:D:1305:MET:HB3	1.87	0.74
1:D:1229:SER:HB3	1:D:1271:VAL:HG12	1.69	0.74
1:A:1280:GLU:O	1:A:1283:ILE:HG22	1.88	0.73
1:A:1328:PRO:O	3:A:1401:HOH:O	2.05	0.73
1:B:1253:THR:O	1:B:1257:TYR:HD1	1.72	0.72
1:D:1209:TRP:HD1	1:D:1236:THR:HA	1.55	0.72
1:A:1317:GLY:HA2	1:A:1340:ASN:HD22	1.54	0.71
1:B:1320:ASP:O	1:B:1338:ARG:NH2	2.22	0.71
1:C:1213:ILE:HG12	1:C:1243:ILE:HD11	1.71	0.71
1:D:1311:MET:HE2	1:D:1346:ILE:HG12	1.74	0.70
1:C:1311:MET:CE	1:C:1346:ILE:HG12	2.22	0.69
1:D:1229:SER:OG	1:D:1328:PRO:O	2.09	0.69
1:D:1324:HIS:CG	1:D:1325:PRO:HD3	2.27	0.69
1:A:1305:MET:CB	1:A:1308:VAL:O	2.38	0.68
1:B:1221:PHE:HE1	1:B:1288:LEU:HD12	1.59	0.68
1:A:1217:SER:CA	1:A:1220:LYS:HE2	2.24	0.68
1:A:1214:ASN:ND2	1:A:1244:GLN:OE1	2.26	0.68
1:C:1324:HIS:CG	1:C:1325:PRO:HD3	2.29	0.68
1:C:1212:PHE:CE1	1:C:1220:LYS:HG2	2.30	0.67
1:D:1327:VAL:H	1:D:1328:PRO:HD2	1.60	0.67
1:A:1306:LYS:HA	1:D:1305:MET:CE	2.24	0.66
1:D:1233:GLU:HB3	1:D:1353:ARG:HD2	1.77	0.66
1:A:1230:GLY:HA3	1:A:1348:ARG:HD2	1.78	0.66
1:D:1225:ALA:HB1	1:D:1272:VAL:HG21	1.77	0.66
1:C:1311:MET:HE3	1:C:1346:ILE:HG12	1.77	0.65
1:A:1278:THR:HG22	1:A:1280:GLU:H	1.61	0.65
1:D:1307:GLN:O	1:D:1348:ARG:HA	1.96	0.65
1:C:1305:MET:O	1:C:1308:VAL:HG12	1.98	0.64
1:A:1208:ILE:HD11	1:A:1232:PRO:HB2	1.80	0.64
1:A:1303:ASN:O	1:A:1305:MET:HG3	1.98	0.64
1:C:1212:PHE:HE1	1:C:1220:LYS:HG2	1.62	0.64
1:D:1229:SER:HB2	1:D:1329:PHE:HD1	1.62	0.64
1:D:1229:SER:HB3	1:D:1271:VAL:CG1	2.27	0.63
1:C:1221:PHE:HB3	1:C:1284:SER:OG	1.98	0.63
1:A:1217:SER:HA	1:A:1220:LYS:HE2	1.81	0.63
1:A:1317:GLY:HA2	1:A:1340:ASN:ND2	2.13	0.63
1:C:1255:TRP:HA	1:C:1258:VAL:HG12	1.80	0.63
1:A:1251:PRO:HB3	1:A:1298:TYR:CD1	2.35	0.62
1:A:1251:PRO:HB3	1:A:1298:TYR:CG	2.36	0.61
1:B:1221:PHE:CE1	1:B:1288:LEU:HD12	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:TYR:CD1	1:A:1345:LEU:HD23	2.35	0.61
1:A:1314:ILE:HD11	1:A:1345:LEU:HB2	1.83	0.61
1:D:1250:SER:O	1:D:1253:THR:HG22	2.00	0.61
1:D:1257:TYR:HB2	2:F:12:PRO:HG3	1.83	0.61
1:D:1235:LEU:O	1:D:1239:LEU:N	2.34	0.60
1:D:1291:TYR:O	1:D:1295:ARG:HD2	2.00	0.60
1:D:1231:SER:OG	1:D:1353:ARG:HD3	2.01	0.60
1:A:1291:TYR:O	1:A:1295:ARG:CG	2.49	0.59
1:A:1249:ILE:O	1:A:1251:PRO:HD3	2.02	0.59
1:B:1327:VAL:HG23	1:B:1328:PRO:CD	2.32	0.59
1:D:1255:TRP:CH2	1:D:1326:LEU:HD11	2.38	0.58
1:C:1237:GLU:O	1:C:1305:MET:HG2	2.02	0.58
1:B:1255:TRP:CH2	1:B:1326:LEU:HD11	2.39	0.58
1:D:1212:PHE:CE1	1:D:1222:VAL:HG22	2.39	0.58
1:D:1324:HIS:CD2	1:D:1325:PRO:HD3	2.39	0.57
1:A:1212:PHE:CE1	1:A:1222:VAL:HG22	2.41	0.56
1:C:1212:PHE:HE1	1:C:1220:LYS:CG	2.17	0.56
1:C:1324:HIS:CD2	1:C:1325:PRO:HD3	2.41	0.56
1:A:1327:VAL:HG23	1:A:1328:PRO:CD	2.33	0.56
1:B:1222:VAL:HG13	1:B:1281:ASP:OD2	2.04	0.56
1:C:1212:PHE:CE1	1:C:1220:LYS:CG	2.89	0.55
1:A:1264:SER:OG	1:A:1267:LYS:HB2	2.06	0.55
1:A:1254:VAL:HG12	1:A:1254:VAL:O	2.07	0.54
1:D:1216:PRO:C	1:D:1217:SER:HG	2.13	0.54
1:D:1235:LEU:HA	1:D:1238:ASP:HB2	1.88	0.54
1:A:1305:MET:CB	1:A:1308:VAL:HG13	2.38	0.53
1:A:1306:LYS:HE3	1:D:1306:LYS:O	2.09	0.53
1:C:1213:ILE:HG12	1:C:1243:ILE:CD1	2.38	0.52
1:D:1314:ILE:HD11	1:D:1345:LEU:HB2	1.91	0.51
1:A:1231:SER:OG	1:A:1351:LEU:O	2.20	0.51
1:A:1251:PRO:HD3	1:A:1297:ARG:HA	1.93	0.50
1:A:1349:GLN:O	1:A:1350:LYS:HB2	2.11	0.50
1:B:1248:ARG:NE	2:F:11:SEP:O1P	2.32	0.50
1:D:1283:ILE:O	1:D:1286:THR:OG1	2.28	0.50
1:A:1283:ILE:O	1:A:1286:THR:OG1	2.28	0.49
1:B:1317:GLY:C	1:B:1338:ARG:NH1	2.61	0.49
1:C:1255:TRP:CZ2	1:C:1323:PRO:HG2	2.46	0.49
1:A:1253:THR:HG21	2:E:9:SER:CB	2.40	0.49
2:F:6:THR:O	2:F:7:SEP:HB3	2.11	0.49
1:A:1251:PRO:HB3	1:A:1298:TYR:CD2	2.48	0.49
1:A:1229:SER:HB2	1:A:1329:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1255:TRP:CZ3	1:D:1326:LEU:HD11	2.48	0.49
1:D:1255:TRP:CZ2	1:D:1323:PRO:HG2	2.48	0.48
1:D:1305:MET:HG3	1:D:1306:LYS:H	1.79	0.48
1:D:1214:ASN:ND2	1:D:1242:SER:OG	2.42	0.48
1:B:1254:VAL:O	1:B:1258:VAL:HG23	2.13	0.48
1:B:1323:PRO:HB2	1:B:1326:LEU:CD1	2.43	0.48
1:C:1213:ILE:HG12	1:C:1243:ILE:CG1	2.43	0.48
1:A:1224:LYS:HG3	1:A:1277:VAL:HG22	1.96	0.47
1:D:1323:PRO:HB2	1:D:1326:LEU:CD1	2.43	0.47
1:A:1295:ARG:HB2	1:A:1297:ARG:HG2	1.96	0.47
1:A:1229:SER:HB2	1:A:1329:PHE:HD1	1.80	0.47
1:A:1298:TYR:CZ	1:A:1314:ILE:HG23	2.49	0.47
1:A:1218:VAL:HG13	1:A:1219:ALA:H	1.79	0.47
1:D:1317:GLY:O	1:D:1338:ARG:NH2	2.38	0.47
1:A:1297:ARG:NH1	2:E:7:SEP:O2P	2.48	0.47
1:D:1237:GLU:HG3	1:D:1354:GLN:HE22	1.80	0.46
1:B:1324:HIS:O	1:B:1327:VAL:HG22	2.16	0.46
1:C:1229:SER:HB2	1:C:1329:PHE:HD1	1.81	0.46
1:B:1311:MET:CE	1:B:1346:ILE:HG12	2.46	0.46
1:A:1219:ALA:CB	1:A:1288:LEU:HB2	2.46	0.46
1:A:1324:HIS:N	1:A:1325:PRO:CD	2.79	0.46
1:C:1250:SER:OG	1:C:1252:GLN:CD	2.59	0.46
1:C:1324:HIS:N	1:C:1325:PRO:CD	2.79	0.46
1:D:1209:TRP:CD1	1:D:1236:THR:HA	2.43	0.46
1:A:1327:VAL:N	1:A:1328:PRO:HD2	2.31	0.45
1:B:1272:VAL:HG13	1:B:1346:ILE:HD11	1.98	0.45
1:B:1327:VAL:N	1:B:1328:PRO:HD2	2.31	0.45
1:C:1218:VAL:O	1:C:1218:VAL:HG23	2.17	0.45
1:B:1334:LEU:HD22	1:B:1334:LEU:N	2.32	0.45
1:A:1233:GLU:HB3	1:A:1353:ARG:HB2	1.99	0.45
1:B:1298:TYR:CZ	1:B:1314:ILE:HG23	2.51	0.45
1:B:1324:HIS:N	1:B:1325:PRO:CD	2.79	0.45
1:C:1316:LEU:HD21	1:C:1338:ARG:NE	2.32	0.45
1:D:1208:ILE:HG12	1:D:1227:PRO:HD3	1.99	0.45
1:A:1306:LYS:HA	1:D:1305:MET:HE1	1.97	0.45
1:B:1255:TRP:CZ3	1:B:1326:LEU:HD11	2.52	0.45
1:A:1231:SER:CB	1:A:1351:LEU:HA	2.47	0.45
1:A:1244:GLN:H	1:A:1303:ASN:HD21	1.65	0.45
1:A:1334:LEU:HD11	1:A:1343:LEU:HD21	1.98	0.45
1:B:1218:VAL:HG23	1:B:1218:VAL:O	2.17	0.45
1:D:1229:SER:HB2	1:D:1329:PHE:CD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1208:ILE:HG12	1:C:1227:PRO:HD3	1.98	0.44
1:D:1208:ILE:HG21	1:D:1232:PRO:O	2.17	0.44
1:A:1251:PRO:HB3	1:A:1298:TYR:CE1	2.52	0.44
1:A:1306:LYS:CG	1:D:1306:LYS:HA	2.48	0.44
1:B:1221:PHE:HB3	1:B:1284:SER:HB2	1.99	0.44
1:C:1298:TYR:CZ	1:C:1314:ILE:HG23	2.52	0.44
1:C:1240:PRO:HA	1:C:1305:MET:HE2	2.00	0.44
1:C:1229:SER:HB2	1:C:1329:PHE:CD1	2.53	0.44
1:B:1222:VAL:CG1	1:B:1281:ASP:OD2	2.66	0.44
1:D:1305:MET:HE3	1:D:1305:MET:HA	1.98	0.44
1:D:1324:HIS:N	1:D:1325:PRO:CD	2.81	0.44
1:D:1214:ASN:OD1	1:D:1220:LYS:HB3	2.18	0.44
2:F:6:THR:O	2:F:7:SEP:CB	2.65	0.44
1:A:1269:ILE:HB	1:A:1346:ILE:O	2.18	0.43
1:A:1229:SER:CB	1:A:1271:VAL:CG1	2.90	0.43
1:B:1351:LEU:HD12	1:D:1217:SER:HB2	1.99	0.43
1:D:1213:ILE:HD12	1:D:1223:THR:HG21	1.99	0.43
1:A:1251:PRO:CD	1:A:1297:ARG:HA	2.49	0.43
1:B:1209:TRP:HA	1:B:1236:THR:HG23	2.00	0.43
1:C:1277:VAL:HG23	1:C:1278:THR:HG23	2.00	0.43
1:D:1238:ASP:O	1:D:1305:MET:CB	2.60	0.43
1:D:1277:VAL:HG23	1:D:1278:THR:HG23	2.01	0.43
1:C:1255:TRP:CH2	1:C:1326:LEU:HD11	2.53	0.43
1:D:1218:VAL:O	1:D:1218:VAL:HG23	2.18	0.43
1:D:1298:TYR:CZ	1:D:1314:ILE:HG23	2.53	0.43
1:C:1327:VAL:N	1:C:1328:PRO:HD2	2.33	0.43
1:D:1288:LEU:HD12	1:D:1288:LEU:HA	1.90	0.43
1:B:1208:ILE:HG12	1:B:1227:PRO:HD3	2.01	0.43
1:A:1235:LEU:O	1:A:1235:LEU:HD23	2.18	0.43
1:A:1255:TRP:HH2	1:A:1298:TYR:HH	1.60	0.42
1:B:1255:TRP:CZ2	1:B:1323:PRO:HG2	2.54	0.42
1:A:1208:ILE:HG12	1:A:1227:PRO:HD3	2.01	0.42
1:A:1269:ILE:HD12	1:A:1269:ILE:O	2.19	0.42
1:D:1250:SER:HB3	1:D:1253:THR:HG22	2.02	0.42
1:A:1208:ILE:HD11	1:A:1232:PRO:CB	2.48	0.42
1:A:1219:ALA:HB3	1:A:1288:LEU:HD13	2.02	0.42
1:C:1232:PRO:HA	1:C:1235:LEU:HD11	2.01	0.42
1:A:1306:LYS:HG3	1:D:1306:LYS:HA	2.01	0.42
1:D:1255:TRP:HZ2	1:D:1298:TYR:OH	2.02	0.42
1:B:1235:LEU:O	1:B:1235:LEU:HD23	2.19	0.42
1:B:1213:ILE:HD12	1:B:1223:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1270:CYS:HB3	1:B:1346:ILE:HB	2.02	0.42
1:D:1213:ILE:HD13	1:D:1313:LEU:HD21	2.02	0.42
1:B:1287:LEU:HD13	1:B:1287:LEU:HA	1.93	0.41
1:B:1305:MET:HB3	1:B:1308:VAL:HG23	2.03	0.41
1:A:1229:SER:OG	1:A:1329:PHE:HA	2.19	0.41
1:B:1239:LEU:HG	1:B:1240:PRO:HD2	2.02	0.41
1:A:1227:PRO:HG3	1:A:1232:PRO:HB3	2.02	0.41
1:B:1255:TRP:HZ2	1:B:1298:TYR:OH	2.04	0.41
1:B:1277:VAL:HG23	1:B:1278:THR:HG23	2.03	0.41
1:A:1217:SER:O	1:A:1220:LYS:CE	2.69	0.41
1:A:1221:PHE:HB3	1:A:1284:SER:HB2	2.02	0.41
1:A:1270:CYS:SG	1:A:1348:ARG:NE	2.91	0.41
1:D:1221:PHE:HB3	1:D:1284:SER:HB2	2.02	0.41
1:D:1232:PRO:O	1:D:1235:LEU:HD12	2.21	0.41
1:A:1248:ARG:HD3	1:C:1309:LYS:HE3	2.02	0.41
1:A:1255:TRP:CZ3	1:A:1326:LEU:HD11	2.55	0.41
1:A:1295:ARG:HG2	1:A:1295:ARG:H	1.75	0.41
1:B:1248:ARG:HB3	1:B:1297:ARG:HD2	2.03	0.41
1:B:1266:THR:O	1:B:1350:LYS:NZ	2.54	0.40
1:A:1251:PRO:CB	1:A:1298:TYR:CE1	3.05	0.40
1:C:1214:ASN:O	1:C:1244:GLN:HA	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:SER:O	1:B:1259:GLU:OE2[1_545]	2.01	0.19

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	147/162 (91%)	124 (84%)	17 (12%)	6 (4%)	2	4
1	B	144/162 (89%)	126 (88%)	11 (8%)	7 (5%)	1	3
1	C	146/162 (90%)	126 (86%)	18 (12%)	2 (1%)	9	19
1	D	147/162 (91%)	131 (89%)	13 (9%)	3 (2%)	6	13
2	E	6/14 (43%)	3 (50%)	2 (33%)	1 (17%)	0	0
2	F	6/14 (43%)	3 (50%)	2 (33%)	1 (17%)	0	0
All	All	596/676 (88%)	513 (86%)	63 (11%)	20 (3%)	3	6

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1236	THR
1	A	1218	VAL
1	A	1250	SER
1	B	1309	LYS
1	B	1352	LYS
1	D	1327	VAL
1	A	1323	PRO
1	B	1232	PRO
1	B	1234	TYR
1	B	1219	ALA
1	C	1219	ALA
1	A	1254	VAL
1	D	1219	ALA
2	E	10	TYR
2	F	8	PRO
1	A	1332	PRO
1	A	1346	ILE
1	B	1339	PRO
1	B	1328	PRO
1	D	1232	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/141 (94%)	125 (95%)	7 (5%)	20	42
1	B	131/141 (93%)	124 (95%)	7 (5%)	20	42
1	C	131/141 (93%)	128 (98%)	3 (2%)	44	68
1	D	132/141 (94%)	129 (98%)	3 (2%)	44	68
2	E	7/10 (70%)	7 (100%)	0	100	100
2	F	7/10 (70%)	7 (100%)	0	100	100
All	All	540/584 (92%)	520 (96%)	20 (4%)	30	55

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1218	VAL
1	A	1220	LYS
1	A	1223	THR
1	A	1295	ARG
1	A	1309	LYS
1	A	1336	LEU
1	A	1346	ILE
1	B	1206	ASN
1	B	1220	LYS
1	B	1223	THR
1	B	1287	LEU
1	B	1288	LEU
1	B	1310	ASP
1	B	1350	LYS
1	C	1212	PHE
1	C	1223	THR
1	C	1279	GLU
1	D	1284	SER
1	D	1297	ARG
1	D	1343	LEU

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	1214	ASN
1	A	1244	GLN
1	A	1340	ASN
1	A	1349	GLN
1	B	1349	GLN

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Mol	Chain	Res	Type
1	B	1354	GLN
1	C	1244	GLN
1	C	1349	GLN
1	D	1307	GLN
1	D	1324	HIS
1	D	1354	GLN

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	$\# Z > 2$
2	SEP	E	7	2	8,9,10	0.56	0	7,12,14	0.87	0
2	SEP	F	14	2	8,9,10	0.76	0	7,12,14	0.71	0
2	SEP	F	11	2	8,9,10	0.64	0	7,12,14	0.82	0
2	SEP	E	11	2	8,9,10	0.71	0	7,12,14	0.77	0
2	SEP	E	14	2	8,9,10	0.66	0	7,12,14	0.68	0
2	SEP	F	7	2	8,9,10	0.61	0	7,12,14	0.69	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
2	SEP	E	7	2	-	2/6/8/10	-
2	SEP	F	14	2	-	4/6/8/10	-
2	SEP	F	11	2	-	2/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	E	11	2	-	4/6/8/10	-
2	SEP	E	14	2	-	4/6/8/10	-
2	SEP	F	7	2	-	3/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	7	SEP	CB-OG-P-O2P
2	F	7	SEP	CB-OG-P-O3P
2	E	11	SEP	N-CA-CB-OG
2	E	11	SEP	C-CA-CB-OG
2	E	11	SEP	CB-OG-P-O2P
2	E	11	SEP	CB-OG-P-O3P
2	F	11	SEP	N-CA-CB-OG
2	F	11	SEP	C-CA-CB-OG
2	E	14	SEP	CB-OG-P-O1P
2	E	14	SEP	CB-OG-P-O2P
2	E	14	SEP	CB-OG-P-O3P
2	F	14	SEP	CA-CB-OG-P
2	F	14	SEP	CB-OG-P-O2P
2	F	14	SEP	CB-OG-P-O3P
2	F	7	SEP	CB-OG-P-O1P
2	E	7	SEP	CA-CB-OG-P
2	E	14	SEP	CA-CB-OG-P
2	E	7	SEP	CB-OG-P-O3P
2	F	14	SEP	CB-OG-P-O1P

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	7	SEP	1	0
2	F	11	SEP	1	0
2	E	14	SEP	1	0
2	F	7	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	149/162 (91%)	-1.41	0 100 100	51, 76, 115, 131	0
1	B	148/162 (91%)	-1.32	0 100 100	36, 77, 116, 132	1 (0%)
1	C	148/162 (91%)	-1.46	0 100 100	49, 71, 106, 126	0
1	D	149/162 (91%)	-1.46	0 100 100	31, 71, 99, 119	1 (0%)
2	E	7/14 (50%)	-1.11	0 100 100	56, 83, 109, 119	0
2	F	7/14 (50%)	-1.22	0 100 100	63, 74, 93, 108	0
All	All	608/676 (89%)	-1.41	0 100 100	31, 74, 111, 132	2 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	SEP	E	7	10/11	0.99	0.03	75,87,90,90	0
2	SEP	F	7	10/11	0.99	0.04	89,94,107,113	0
2	SEP	E	11	10/11	0.99	0.03	83,92,95,103	0
2	SEP	F	11	10/11	0.99	0.03	67,75,77,78	0
2	SEP	F	14	10/11	0.99	0.03	59,67,74,77	0
2	SEP	E	14	10/11	1.00	0.03	47,53,60,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.