



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:17 AM UTC

PDB ID : 3F7P / pdb_00003f7p
Title : Crystal structure of a complex between integrin beta4 and plectin
Authors : de Pereda, J.M.
Deposited on : 2008-11-10
Resolution : 2.75 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

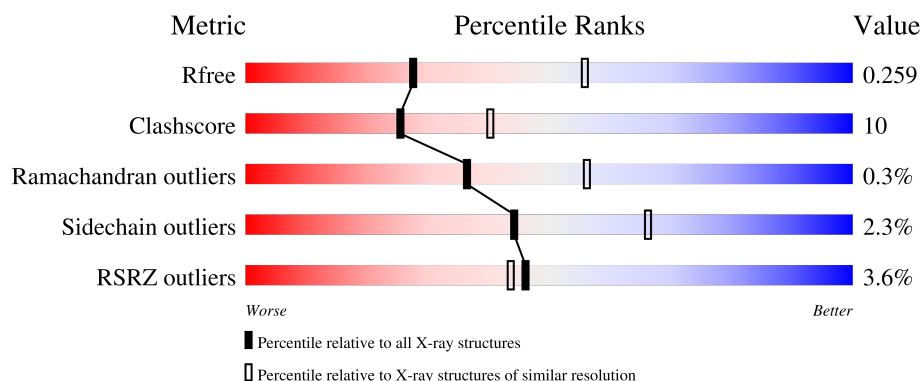
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	296	0% 65% 12% 22%
1	B	296	2% 63% 13% 22%
2	C	248	4% 59% 21% 19%
2	D	248	2% 54% 24% 21%
2	E	248	5% 62% 23% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8564 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 Plectin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1897	1195	346	350	6			
1	B	230	Total	C	N	O	S	0	0	0
			1892	1192	345	349	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q15149
A	-1	SER	-	expression tag	UNP Q15149
A	0	HIS	-	expression tag	UNP Q15149
B	-2	GLY	-	expression tag	UNP Q15149
B	-1	SER	-	expression tag	UNP Q15149
B	0	HIS	-	expression tag	UNP Q15149

- Molecule 2 is a protein called Integrin beta-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	200	Total	C	N	O	S	0	0	0
			1556	982	270	296	8			
2	D	196	Total	C	N	O	S	0	0	0
			1529	964	265	292	8			
2	E	212	Total	C	N	O	S	0	0	0
			1654	1041	283	321	9			

There are 9 discrepancies between the modelled and reference sequences:

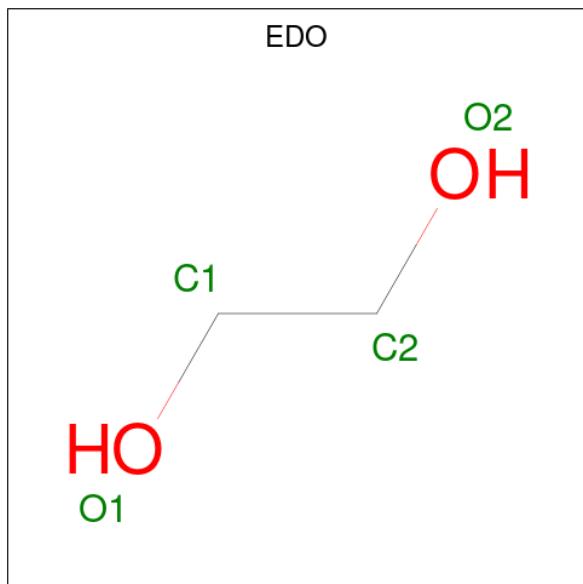
Chain	Residue	Modelled	Actual	Comment	Reference
C	1123	GLY	-	expression tag	UNP P16144
C	1124	SER	-	expression tag	UNP P16144
C	1125	HIS	-	expression tag	UNP P16144
D	1123	GLY	-	expression tag	UNP P16144

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1124	SER	-	expression tag	UNP P16144
D	1125	HIS	-	expression tag	UNP P16144
E	1123	GLY	-	expression tag	UNP P16144
E	1124	SER	-	expression tag	UNP P16144
E	1125	HIS	-	expression tag	UNP P16144

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

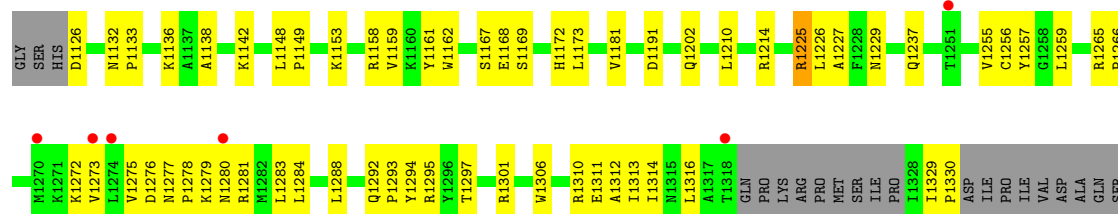
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	3	Total	O	0	0
			3	3		
6	C	3	Total	O	0	0
			3	3		
6	D	3	Total	O	0	0
			3	3		
6	E	3	Total	O	0	0
			3	3		

- Molecule 1: Plectin-1



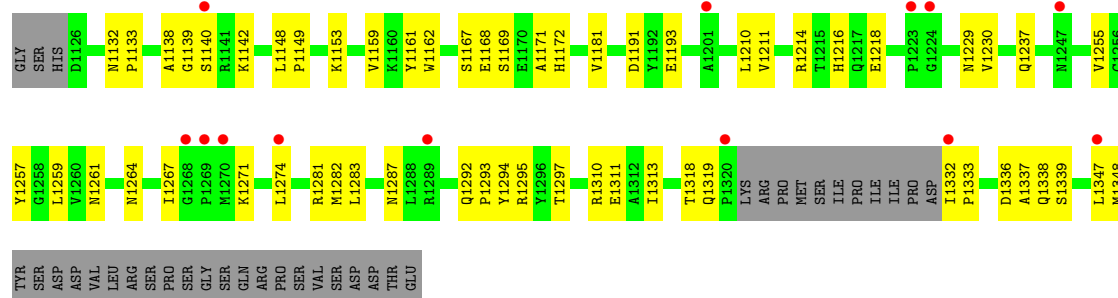
ASP
SER
PHE
LEU
MET
TYR
SER
ASP
VAL
LEU
ARG
SER
PRO
SER
GLY
SER
GLN
ARG
PRO
SER
VAL
SER
SER
ASP
ASP
THR
GLU

● Molecule 2: Integrin beta-4



GLY
GLU
ASP
TYR
SER
PHE
LEU
MET
TYR
SER
ASP
VAL
ARG
SER
PRO
SER
GLY
SER
GLN
ARG
PRO
SER
VAL
SER
ASP
THR
GLU

● Molecule 2: Integrin beta-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.25Å 107.25Å 203.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.53 – 2.75 84.53 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (84.53-2.75) 99.8 (84.53-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.204 , 0.257 0.208 , 0.259	Depositor DCC
R_{free} test set	1897 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8564	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: PEG, EDO, CA

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	0.43	0/1931	0.79	3/2608 (0.1%)
1	B	0.39	0/1925	0.76	4/2598 (0.2%)
2	C	0.39	0/1596	0.87	8/2174 (0.4%)
2	D	0.38	0/1568	0.78	2/2135 (0.1%)
2	E	0.40	0/1696	0.82	4/2309 (0.2%)
All	All	0.40	0/8716	0.80	21/11824 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1289	ARG	NE-CZ-NH2	9.66	127.90	119.20
2	C	1289	ARG	NE-CZ-NH1	-9.35	112.15	121.50
2	C	1281	ARG	NE-CZ-NH2	8.32	126.69	119.20
2	C	1281	ARG	NE-CZ-NH1	-8.23	113.27	121.50
1	A	148	ARG	NE-CZ-NH2	7.86	126.28	119.20
2	C	1289	ARG	CD-NE-CZ	7.55	134.97	124.40
1	A	148	ARG	NE-CZ-NH1	-7.50	114.00	121.50
1	B	148	ARG	NE-CZ-NH2	-6.14	113.67	119.20
2	C	1281	ARG	CD-NE-CZ	5.80	132.52	124.40
2	E	1281	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	A	148	ARG	CD-NE-CZ	5.72	132.41	124.40
2	E	1281	ARG	CD-NE-CZ	5.63	132.28	124.40
1	B	156	ASN	CA-C-N	5.52	124.71	118.97
1	B	156	ASN	C-N-CA	5.52	124.71	118.97
2	D	1153	LYS	CA-C-N	5.49	125.42	119.76
2	D	1153	LYS	C-N-CA	5.49	125.42	119.76
1	B	148	ARG	CD-NE-CZ	5.41	131.97	124.40
2	C	1153	LYS	CA-C-N	5.13	124.89	119.76
2	C	1153	LYS	C-N-CA	5.13	124.89	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1153	LYS	CA-C-N	5.00	124.76	119.76
2	E	1153	LYS	C-N-CA	5.00	124.76	119.76

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	1897	0	1915	27	0
1	B	1892	0	1909	35	0
2	C	1556	0	1520	35	0
2	D	1529	0	1491	49	0
2	E	1654	0	1597	37	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	B	7	0	10	1	0
5	D	1	0	0	0	0
6	A	8	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	D	3	0	0	0	0
6	E	3	0	0	0	0
All	All	8564	0	8454	163	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 10.

All (163) 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)
2:C:1177:LYS:HZ1	2:D:1272:LYS:HE3	1.17	1.06
1:B:61:ILE:HD13	2:D:1273:VAL:HG21	1.54	0.89
2:C:1177:LYS:NZ	2:D:1272:LYS:HE3	1.91	0.86
1:B:61:ILE:HD11	2:D:1283:LEU:HD21	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLU:O	1:B:98:ARG:HG3	1.82	0.80
1:A:95:GLU:O	1:A:98:ARG:HG3	1.81	0.79
1:A:239:ARG:HA	2:E:1211:VAL:HG23	1.67	0.76
2:C:1177:LYS:HZ1	2:D:1272:LYS:CE	2.00	0.71
2:E:1271:LYS:HE3	2:E:1337:ALA:O	1.91	0.70
1:A:158:LYS:HE2	2:C:1229:ASN:ND2	2.07	0.70
2:E:1336:ASP:HB3	2:E:1339:SER:HB3	1.76	0.68
2:D:1138:ALA:O	2:D:1142:LYS:HG3	1.93	0.68
2:E:1140:SER:CB	2:E:1218:GLU:HG2	2.25	0.67
2:C:1138:ALA:O	2:C:1142:LYS:HG3	1.95	0.66
2:E:1138:ALA:O	2:E:1142:LYS:HG3	1.96	0.66
2:D:1167:SER:C	2:D:1169:SER:H	2.05	0.64
1:B:61:ILE:HD11	2:D:1283:LEU:CD2	2.26	0.64
1:B:66:GLU:HA	1:B:69:ARG:HG3	1.79	0.63
2:C:1167:SER:C	2:C:1169:SER:H	2.05	0.63
2:D:1229:ASN:HB2	2:D:1237:GLN:HB3	1.81	0.62
2:C:1189:TYR:CG	2:C:1248:GLY:HA2	2.34	0.62
1:A:197:ARG:HH11	1:A:197:ARG:HG2	1.64	0.61
1:B:197:ARG:HG2	1:B:197:ARG:HH11	1.65	0.61
2:E:1167:SER:C	2:E:1169:SER:H	2.06	0.61
2:E:1140:SER:HB2	2:E:1218:GLU:HG2	1.82	0.61
2:C:1314:ILE:HD11	2:C:1330:PRO:HG3	1.82	0.61
2:D:1132:ASN:N	2:D:1133:PRO:HD3	2.16	0.60
2:E:1261:ASN:HB3	2:E:1267:ILE:HG21	1.82	0.60
2:E:1287:ASN:O	2:E:1338:GLN:HG2	2.02	0.60
1:B:173:ILE:O	1:B:176:ILE:HG12	2.02	0.60
1:B:69:ARG:O	1:B:73:LYS:HG3	2.04	0.58
2:D:1312:ALA:HB1	2:D:1330:PRO:HG2	1.86	0.58
1:B:95:GLU:HB2	2:D:1279:LYS:CE	2.35	0.57
1:A:173:ILE:O	1:A:176:ILE:HG12	2.04	0.57
2:C:1148:LEU:HD12	2:C:1149:PRO:HD2	1.85	0.57
2:D:1259:LEU:O	2:D:1266:PRO:HA	2.04	0.57
2:D:1255:VAL:HG21	2:D:1283:LEU:HD22	1.87	0.56
2:E:1229:ASN:HB2	2:E:1237:GLN:HB3	1.86	0.56
2:C:1287:ASN:CG	2:C:1287:ASN:O	2.48	0.56
2:C:1255:VAL:HG21	2:C:1283:LEU:HD22	1.88	0.56
2:C:1158:ARG:NH2	2:C:1173:LEU:HD13	2.21	0.55
2:C:1191:ASP:OD1	2:C:1214:ARG:HB2	2.07	0.55
1:B:61:ILE:CD1	2:D:1273:VAL:HG21	2.31	0.55
1:B:95:GLU:HB2	2:D:1279:LYS:HE2	1.89	0.55
2:D:1226:LEU:O	2:D:1329:ILE:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:VAL:HG22	1:B:146:ASN:HB2	1.89	0.55
2:D:1191:ASP:OD1	2:D:1214:ARG:HB2	2.07	0.55
2:E:1148:LEU:HD12	2:E:1149:PRO:HD2	1.89	0.55
1:B:120:GLY:HA3	1:B:125:HIS:CG	2.42	0.54
1:B:236:LYS:HE3	1:B:240:GLN:OE1	2.08	0.54
2:D:1301:ARG:HB2	2:D:1306:TRP:CD2	2.42	0.54
1:A:67:ARG:HA	1:A:70:VAL:CG1	2.38	0.53
1:B:67:ARG:HA	1:B:70:VAL:CG1	2.39	0.53
1:A:62:ARG:HH11	1:A:62:ARG:HG3	1.72	0.53
1:A:62:ARG:HG3	1:A:62:ARG:NH1	2.24	0.53
2:C:1225:ARG:NH1	2:C:1329:ILE:HG21	2.24	0.53
2:C:1132:ASN:N	2:C:1133:PRO:HD3	2.23	0.53
2:E:1191:ASP:OD1	2:E:1214:ARG:HB2	2.08	0.53
2:E:1230:VAL:HG21	2:E:1319:GLN:HB2	1.91	0.52
2:E:1257:TYR:HA	2:E:1295:ARG:O	2.09	0.52
1:A:120:GLY:HA3	1:A:125:HIS:CG	2.44	0.52
1:B:62:ARG:HE	2:D:1284:LEU:HD23	1.75	0.52
2:C:1189:TYR:CD2	2:C:1248:GLY:HA2	2.45	0.52
2:D:1259:LEU:HD22	2:D:1294:TYR:CE2	2.45	0.52
2:E:1259:LEU:HD22	2:E:1294:TYR:CE2	2.46	0.51
2:D:1148:LEU:HD12	2:D:1149:PRO:HD2	1.91	0.51
1:B:66:GLU:O	1:B:70:VAL:HG12	2.11	0.51
2:D:1257:TYR:HA	2:D:1295:ARG:O	2.11	0.51
2:E:1274:LEU:HB2	2:E:1347:LEU:HD12	1.93	0.51
1:A:236:LYS:HE3	1:A:240:GLN:OE1	2.11	0.50
2:C:1167:SER:C	2:C:1169:SER:N	2.70	0.50
1:B:182:SER:HB2	1:B:185:MET:HG3	1.94	0.50
2:C:1259:LEU:HD22	2:C:1294:TYR:CE2	2.46	0.50
2:E:1132:ASN:N	2:E:1133:PRO:HD3	2.27	0.50
1:B:202:TYR:HB3	1:B:205:LEU:HD22	1.94	0.49
2:D:1277:ASN:HB3	2:D:1280:ASN:OD1	2.12	0.49
2:D:1314:ILE:HD11	2:D:1330:PRO:HG3	1.94	0.49
1:A:197:ARG:HH11	1:A:197:ARG:CG	2.25	0.49
2:D:1126:ASP:HB3	2:D:1202:GLN:OE1	2.13	0.49
1:B:61:ILE:HG12	1:B:62:ARG:N	2.29	0.48
1:A:202:TYR:HB3	1:A:205:LEU:HD22	1.95	0.48
2:C:1319:GLN:HG3	2:C:1328:ILE:HD13	1.96	0.48
1:A:243:LEU:HD11	2:E:1214:ARG:HH12	1.80	0.47
2:C:1158:ARG:CZ	2:D:1295:ARG:NH2	2.77	0.47
1:A:61:ILE:HD11	2:E:1347:LEU:HD13	1.96	0.47
1:A:225:HIS:CD2	1:A:229:PRO:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1255:VAL:HG21	2:E:1283:LEU:HD22	1.95	0.47
2:C:1295:ARG:HB2	2:C:1313:ILE:HD13	1.96	0.47
2:E:1230:VAL:HG21	2:E:1319:GLN:CB	2.45	0.47
2:E:1282:MET:HG2	2:E:1332:ILE:HD13	1.97	0.47
4:B:295:PEG:H12	4:B:295:PEG:H31	1.70	0.46
2:C:1141:ARG:HG2	2:C:1186:LEU:O	2.14	0.46
2:E:1140:SER:OG	2:E:1218:GLU:OE2	2.33	0.46
1:A:67:ARG:HA	1:A:70:VAL:HG12	1.97	0.46
2:E:1167:SER:C	2:E:1169:SER:N	2.71	0.46
2:D:1295:ARG:HD2	2:D:1311:GLU:OE2	2.16	0.46
1:A:66:GLU:O	1:A:70:VAL:HG12	2.15	0.46
1:B:157:PRO:CG	2:D:1281:ARG:HB2	2.45	0.46
2:C:1257:TYR:HA	2:C:1295:ARG:O	2.15	0.46
2:C:1301:ARG:HB2	2:C:1306:TRP:CE3	2.50	0.46
2:D:1295:ARG:HB2	2:D:1313:ILE:HD13	1.96	0.46
1:B:248:GLN:O	1:B:252:VAL:HG23	2.16	0.46
1:B:75:PHE:O	1:B:79:VAL:HG23	2.16	0.46
2:E:1162:TRP:HH2	2:E:1210:LEU:HD11	1.81	0.46
2:C:1177:LYS:NZ	2:D:1272:LYS:CE	2.71	0.45
2:D:1276:ASP:O	2:D:1278:PRO:HD3	2.16	0.45
1:B:61:ILE:CD1	2:D:1283:LEU:HD21	2.37	0.45
2:D:1159:VAL:HG21	2:D:1181:VAL:HG11	1.98	0.45
1:B:67:ARG:HA	1:B:70:VAL:HG12	1.99	0.45
2:E:1140:SER:OG	2:E:1218:GLU:CG	2.64	0.45
2:D:1162:TRP:HH2	2:D:1210:LEU:HD11	1.82	0.45
2:C:1159:VAL:HG21	2:C:1181:VAL:HG11	1.98	0.44
2:C:1266:PRO:CG	2:C:1295:ARG:NH1	2.80	0.44
1:B:156:ASN:HA	1:B:157:PRO:HD3	1.79	0.44
2:C:1189:TYR:CD1	2:C:1217:GLN:HG2	2.53	0.44
2:D:1161:TYR:CE1	2:D:1172:HIS:HB2	2.53	0.44
2:E:1139:GLY:C	2:E:1216:HIS:HB2	2.42	0.44
2:C:1162:TRP:HH2	2:C:1210:LEU:HD11	1.81	0.44
2:C:1291:SER:HA	2:C:1317:ALA:HB3	1.99	0.44
1:A:99:ASP:HA	1:A:126:LYS:HG2	1.99	0.43
1:A:95:GLU:OE2	2:C:1281:ARG:NH1	2.43	0.43
1:B:197:ARG:HH11	1:B:197:ARG:CG	2.29	0.43
1:B:225:HIS:CD2	1:B:229:PRO:HA	2.54	0.43
1:A:142:VAL:HG22	1:A:170:HIS:CD2	2.54	0.43
2:C:1297:THR:HA	2:C:1310:ARG:O	2.19	0.43
2:E:1297:THR:HA	2:E:1310:ARG:O	2.18	0.43
2:D:1275:VAL:HG11	2:D:1280:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:HG22	1:B:170:HIS:CD2	2.54	0.43
2:E:1162:TRP:HB3	2:E:1171:ALA:HA	2.01	0.42
1:A:68:ASP:OD1	1:A:158:LYS:NZ	2.52	0.42
2:C:1295:ARG:HD2	2:C:1311:GLU:OE2	2.20	0.42
1:A:182:SER:HB2	1:A:185:MET:HG3	2.00	0.42
2:C:1312:ALA:HB1	2:C:1330:PRO:HG2	2.01	0.42
2:D:1227:ALA:HA	2:D:1329:ILE:HG12	2.01	0.42
2:E:1333:PRO:HB2	2:E:1348:MET:HE2	2.02	0.42
1:A:173:ILE:O	1:A:187:ALA:HB1	2.19	0.42
1:A:173:ILE:HD13	1:A:279:ILE:HG22	2.02	0.42
2:D:1136:LYS:HE3	2:D:1136:LYS:HB2	1.82	0.42
2:D:1297:THR:HA	2:D:1310:ARG:O	2.19	0.42
2:E:1161:TYR:CE1	2:E:1172:HIS:HB2	2.55	0.42
2:E:1162:TRP:CE2	2:E:1193:GLU:HB2	2.53	0.42
2:E:1295:ARG:HD2	2:E:1311:GLU:OE2	2.20	0.42
2:E:1159:VAL:HG21	2:E:1181:VAL:HG11	2.01	0.41
1:B:61:ILE:HD11	2:D:1283:LEU:CG	2.50	0.41
1:A:134:LEU:HD22	1:A:144:LEU:HD13	2.02	0.41
2:D:1225:ARG:HG3	2:D:1329:ILE:HG21	2.03	0.41
2:E:1292:GLN:HA	2:E:1293:PRO:HD3	1.85	0.41
1:B:98:ARG:HE	1:B:98:ARG:HB3	1.69	0.41
2:D:1292:GLN:HA	2:D:1293:PRO:HD3	1.88	0.41
2:E:1295:ARG:HB2	2:E:1313:ILE:HD13	2.02	0.41
1:B:139:HIS:C	1:B:141:GLN:H	2.29	0.41
1:A:236:LYS:HE2	1:A:236:LYS:HB3	1.87	0.41
1:B:65:ASP:HB2	2:D:1284:LEU:HD22	2.03	0.41
2:D:1288:LEU:CD1	2:D:1316:LEU:HD11	2.51	0.41
2:E:1287:ASN:HB2	2:E:1336:ASP:OD1	2.21	0.41
1:A:75:PHE:O	1:A:79:VAL:HG23	2.21	0.41
1:B:173:ILE:O	1:B:173:ILE:HG22	2.21	0.41
2:D:1256:CYS:SG	2:D:1272:LYS:HG2	2.60	0.41
2:C:1235:VAL:HG22	2:C:1286:GLU:CB	2.52	0.40
1:B:99:ASP:HA	1:B:126:LYS:HG2	2.04	0.40
2:D:1158:ARG:NH2	2:D:1173:LEU:HD13	2.36	0.40
2:D:1167:SER:C	2:D:1169:SER:N	2.70	0.40
2:D:1279:LYS:HD2	2:D:1279:LYS:HA	1.97	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	229/296 (77%)	221 (96%)	8 (4%)	0	100	100
1	B	226/296 (76%)	219 (97%)	7 (3%)	0	100	100
2	C	196/248 (79%)	191 (97%)	4 (2%)	1 (0%)	24	43
2	D	192/248 (77%)	187 (97%)	4 (2%)	1 (0%)	24	43
2	E	208/248 (84%)	199 (96%)	8 (4%)	1 (0%)	24	43
All	All	1051/1336 (79%)	1017 (97%)	31 (3%)	3 (0%)	36	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1168	GLU
2	E	1168	GLU
2	C	1168	GLU

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	212/261 (81%)	204 (96%)	8 (4%)	29	52
1	B	212/261 (81%)	204 (96%)	8 (4%)	29	52
2	C	169/214 (79%)	167 (99%)	2 (1%)	63	78
2	D	166/214 (78%)	164 (99%)	2 (1%)	63	78
2	E	180/214 (84%)	178 (99%)	2 (1%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	939/1164 (81%)	917 (98%)	22 (2%)	44 66

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ILE
1	A	63	ILE
1	A	70	VAL
1	A	98	ARG
1	A	128	GLN
1	A	166	THR
1	A	178	VAL
1	A	183	GLU
1	B	61	ILE
1	B	63	ILE
1	B	70	VAL
1	B	98	ARG
1	B	128	GLN
1	B	166	THR
1	B	178	VAL
1	B	183	GLU
2	C	1265	ARG
2	C	1287	ASN
2	D	1225	ARG
2	D	1265	ARG
2	E	1264	ASN
2	E	1318	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	170	HIS
1	A	248	GLN
1	B	82	HIS
1	B	101	HIS
1	B	170	HIS
1	B	248	GLN
1	B	272	GLN
2	C	1237	GLN
2	C	1277	ASN

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Mol	Chain	Res	Type
2	C	1280	ASN
2	D	1229	ASN
2	D	1237	GLN
2	E	1277	ASN
2	E	1319	GLN

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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	EDO	B	294	-	3,3,3	0.49	0	2,2,2	0.48	0
4	PEG	B	295	-	6,6,6	0.77	0	5,5,5	0.93	0
3	EDO	A	294	-	3,3,3	0.53	0	2,2,2	0.55	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	B	294	-	-	0/1/1/1	-
4	PEG	B	295	-	-	1/4/4/4	-
3	EDO	A	294	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	295	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	295	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	231/296 (78%)	-0.12	4 (1%) 69 67	35, 59, 121, 171	0
1	B	230/296 (77%)	0.06	6 (2%) 57 55	45, 76, 128, 153	0
2	C	200/248 (80%)	0.38	10 (5%) 34 34	43, 88, 148, 171	0
2	D	196/248 (79%)	0.38	6 (3%) 51 49	43, 85, 130, 147	0
2	E	212/248 (85%)	0.54	13 (6%) 27 27	46, 82, 137, 165	0
All	All	1069/1336 (80%)	0.24	39 (3%) 46 44	35, 77, 133, 171	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	ILE	5.4
2	E	1140	SER	5.3
1	A	64	ALA	4.6
1	B	290	PRO	4.2
2	E	1320	PRO	4.1
1	B	60	VAL	4.0
2	D	1270	MET	3.4
2	C	1132	ASN	3.3
2	C	1267	ILE	3.1
2	C	1147	TRP	3.0
2	D	1280	ASN	2.9
1	A	63	ILE	2.9
2	E	1347	LEU	2.8
2	E	1269	PRO	2.8
2	E	1201	ALA	2.8
2	D	1274	LEU	2.7
2	C	1291	SER	2.7
2	C	1127	LEU	2.7
2	E	1270	MET	2.6
2	E	1332	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	60	VAL	2.4
2	E	1268	GLY	2.4
1	B	176	ILE	2.4
2	E	1274	LEU	2.3
2	E	1247	ASN	2.3
2	C	1270	MET	2.3
2	C	1181	VAL	2.2
2	C	1148	LEU	2.2
2	D	1273	VAL	2.2
1	B	61	ILE	2.2
2	D	1251	THR	2.2
2	E	1224	GLY	2.1
2	C	1198	ALA	2.1
2	C	1189	TYR	2.1
1	A	124	PHE	2.1
1	B	245	ASN	2.1
2	E	1289	ARG	2.0
2	D	1318	THR	2.0
2	E	1223	PRO	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($\text{\AA}^2$)	Q<0.9
4	PEG	B	295	7/7	0.79	0.17	53,74,87,89	0
3	EDO	A	294	4/4	0.86	0.19	46,57,63,91	0
3	EDO	B	294	4/4	0.87	0.12	60,69,78,80	0
5	CA	D	101	1/1	0.94	0.29	43,43,43,43	1

6.5 Other polymers [i](#)

There are no such residues in this entry.