



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 03:04 PM EDT

PDB ID : 3F7P  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

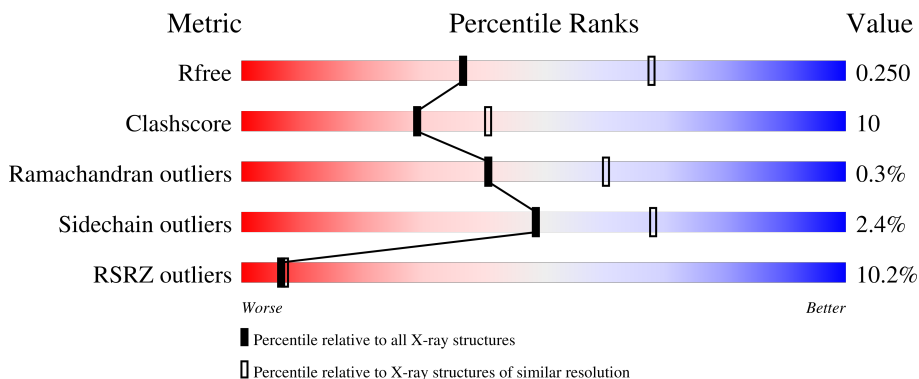
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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	
1	B	296	
2	C	248	
2	D	248	
2	E	248	

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	231	1897	1195	346	350	6	0	0	0
1	B	230	1892	1192	345	349	6	0	0	0

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
			Total	C	N	O	S			
2	C	200	1556	982	270	296	8	0	0	0
2	D	196	1529	964	265	292	8	0	0	0
2	E	212	1654	1041	283	321	9	0	0	0

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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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 (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

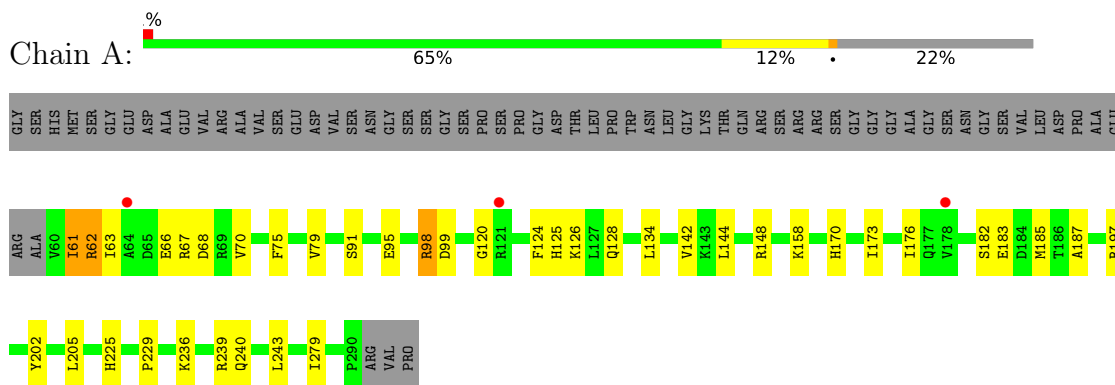
- Molecule 6 is water.

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

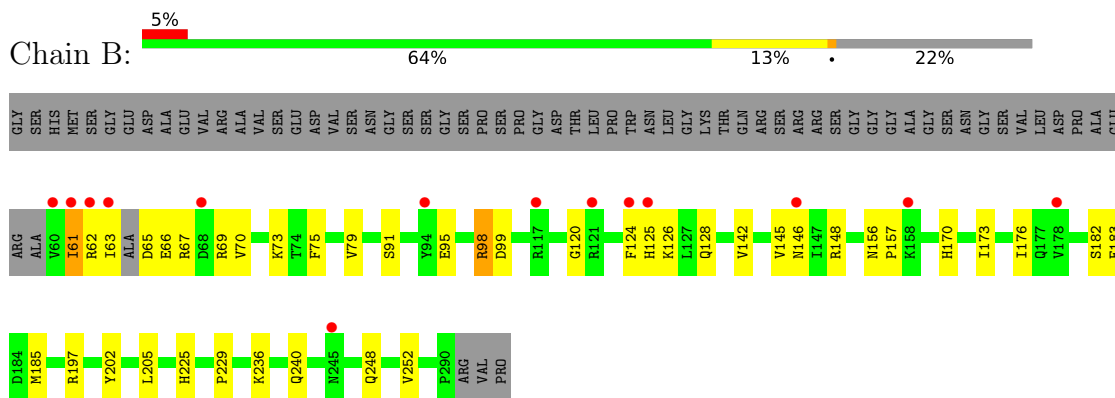
### 3 Residue-property plots [i](#)

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

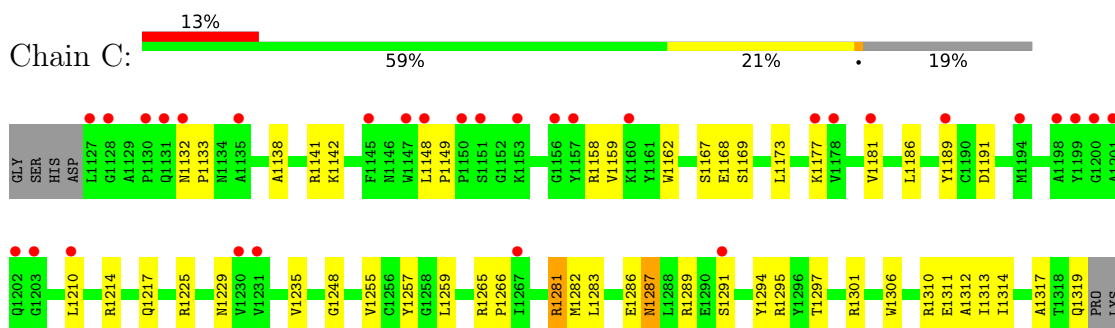
- Molecule 1: Plectin-1

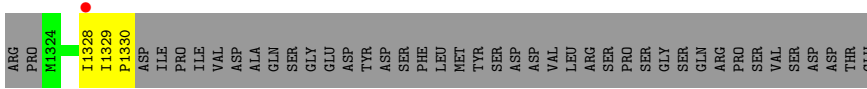


- Molecule 1: Plectin-1

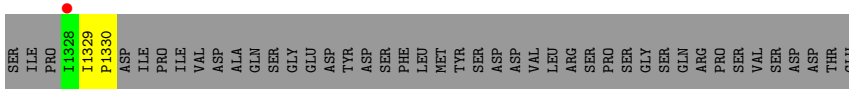
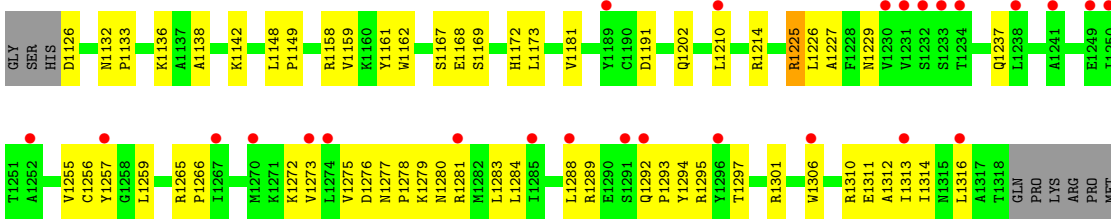


- Molecule 2: Integrin beta-4

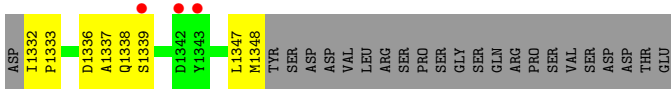
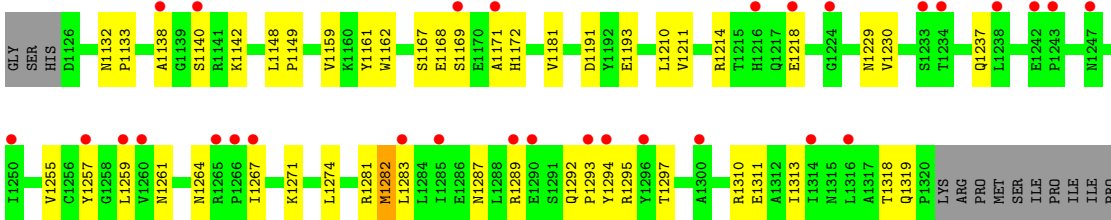




• Molecule 2: Integrin beta-4



• Molecule 2: Integrin beta-4



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.25Å 107.25Å 203.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.53 – 2.75 84.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (84.53-2.75) 99.8 (84.53-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.204 , 0.257 0.197 , 0.250	Depositor DCC
$R_{free}$ test set	1897 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtrriage
Anisotropy	0.395	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.33	0/1931	0.60	3/2608 (0.1%)
1	B	0.31	0/1925	0.59	3/2598 (0.1%)
2	C	0.33	0/1596	0.83	6/2174 (0.3%)
2	D	0.31	0/1568	0.55	2/2135 (0.1%)
2	E	0.32	0/1696	0.70	5/2309 (0.2%)
All	All	0.32	0/8716	0.66	19/11824 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1289	ARG	NE-CZ-NH1	-16.30	112.15	120.30
2	C	1289	ARG	NE-CZ-NH2	15.20	127.90	120.30
2	C	1281	ARG	NE-CZ-NH1	-14.06	113.27	120.30
1	B	148	ARG	NE-CZ-NH2	-13.26	113.67	120.30
2	C	1281	ARG	NE-CZ-NH2	12.78	126.69	120.30
2	E	1281	ARG	NE-CZ-NH2	-12.61	113.99	120.30
1	A	148	ARG	NE-CZ-NH1	-12.60	114.00	120.30
2	E	1281	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	B	148	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	A	148	ARG	NE-CZ-NH2	11.95	126.28	120.30
2	E	1289	ARG	NE-CZ-NH2	-10.06	115.27	120.30
2	E	1289	ARG	NE-CZ-NH1	9.19	124.89	120.30
2	D	1289	ARG	NE-CZ-NH2	-8.87	115.87	120.30
2	D	1289	ARG	NE-CZ-NH1	8.84	124.72	120.30
2	C	1289	ARG	CD-NE-CZ	8.12	134.97	123.60
2	C	1281	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	148	ARG	CD-NE-CZ	6.30	132.41	123.60
2	E	1281	ARG	CD-NE-CZ	6.20	132.28	123.60
1	B	148	ARG	CD-NE-CZ	5.98	131.97	123.60

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	28	0
1	B	1892	0	1909	34	0
2	C	1556	0	1520	36	0
2	D	1529	0	1491	50	0
2	E	1654	0	1597	36	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)
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
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: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:C:1177:LYS:HZ1	2:D:1272:LYS:HE3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1177:LYS:HZ2	2:D:1272:LYS:HE3	1.60	0.65
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: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: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
2:D:1167:SER:C	2:D:1169:SER:H	2.05	0.59
2:C:1167:SER:C	2:C:1169:SER:H	2.05	0.59
2:C:1177:LYS:HZ1	2:D:1272:LYS:CE	2.16	0.58
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:E:1167:SER:C	2:E:1169:SER:H	2.06	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1287:ASN:CG	2:C:1287:ASN:O	2.48	0.51
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1295:ARG:HD2	2:D:1311:GLU:OE2	2.16	0.46
2:E:1333:PRO:HB2	2:E:1348:MET:HE2	1.96	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:C:1167:SER:C	2:C:1169:SER:N	2.70	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: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
2:D:1167:SER:C	2:D:1169:SER:N	2.70	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
2:E:1167:SER:C	2:E:1169:SER:N	2.71	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:173:ILE:O	1:A:173:ILE:HG22	2.21	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: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%)	29	47
2	D	192/248 (77%)	187 (97%)	4 (2%)	1 (0%)	29	47
2	E	208/248 (84%)	199 (96%)	8 (4%)	1 (0%)	29	47
All	All	1051/1336 (79%)	1017 (97%)	31 (3%)	3 (0%)	41	60

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 [i](#)

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%)	33	53
1	B	212/261 (81%)	205 (97%)	7 (3%)	38	58
2	C	169/214 (79%)	166 (98%)	3 (2%)	59	75
2	D	166/214 (78%)	164 (99%)	2 (1%)	71	82
2	E	180/214 (84%)	177 (98%)	3 (2%)	60	76
All	All	939/1164 (81%)	916 (98%)	23 (2%)	49	68

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ILE
1	A	62	ARG

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Mol	Chain	Res	Type
1	A	63	ILE
1	A	91	SER
1	A	98	ARG
1	A	124	PHE
1	A	128	GLN
1	A	183	GLU
1	B	61	ILE
1	B	63	ILE
1	B	91	SER
1	B	98	ARG
1	B	124	PHE
1	B	128	GLN
1	B	183	GLU
2	C	1265	ARG
2	C	1282	MET
2	C	1287	ASN
2	D	1225	ARG
2	D	1265	ARG
2	E	1264	ASN
2	E	1282	MET
2	E	1318	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	170	HIS
1	B	101	HIS
1	B	170	HIS
2	C	1237	GLN
2	D	1229	ASN

### 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 monosaccharides 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
4	PEG	B	295	-	6,6,6	0.77	0	5,5,5	0.94	0
3	EDO	B	294	-	3,3,3	0.53	0	2,2,2	0.45	0
3	EDO	A	294	-	3,3,3	0.57	0	2,2,2	0.53	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
4	PEG	B	295	-	-	1/4/4/4	-
3	EDO	B	294	-	-	0/1/1/1	-
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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	231/296 (78%)	0.44	3 (1%) 77 84	35, 59, 121, 171	0
1	B	230/296 (77%)	0.65	14 (6%) 21 26	45, 76, 128, 153	0
2	C	200/248 (80%)	0.94	32 (16%) 1 2	43, 88, 148, 171	0
2	D	196/248 (79%)	0.98	27 (13%) 2 3	43, 85, 130, 147	0
2	E	212/248 (85%)	1.02	33 (15%) 2 2	46, 82, 137, 165	0
All	All	1069/1336 (80%)	0.79	109 (10%) 6 7	35, 77, 133, 171	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1127	LEU	6.4
2	C	1147	TRP	6.4
2	C	1181	VAL	5.6
2	E	1234	THR	5.6
2	E	1289	ARG	5.5
2	E	1265	ARG	5.2
2	C	1200	GLY	5.1
2	E	1266	PRO	4.9
2	E	1140	SER	4.8
2	C	1201	ALA	4.8
2	D	1274	LEU	4.7
2	D	1288	LEU	4.7
2	D	1232	SER	4.4
2	E	1316	LEU	4.3
1	B	61	ILE	4.3
1	B	63	ILE	4.2
2	C	1153	LYS	4.1
2	E	1224	GLY	4.1
2	C	1199	TYR	3.9
2	E	1233	SER	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	1234	THR	3.9
2	C	1131	GLN	3.9
2	D	1233	SER	3.9
1	B	60	VAL	3.9
1	B	62	ARG	3.7
2	D	1296	TYR	3.7
1	B	68	ASP	3.6
2	D	1230	VAL	3.4
2	C	1148	LEU	3.4
2	D	1231	VAL	3.4
2	E	1285	ILE	3.3
2	C	1203	GLY	3.2
2	E	1294	TYR	3.2
2	D	1291	SER	3.2
2	E	1267	ILE	3.1
2	E	1339	SER	3.0
2	E	1260	VAL	3.0
2	D	1281	ARG	2.9
2	C	1132	ASN	2.9
2	E	1296	TYR	2.9
2	E	1257	TYR	2.9
2	D	1313	ILE	2.9
1	A	121	ARG	2.9
2	C	1130	PRO	2.9
1	B	124	PHE	2.8
2	E	1238	LEU	2.8
2	E	1314	ILE	2.7
2	D	1292	GLN	2.7
2	D	1189	TYR	2.7
2	E	1343	TYR	2.7
2	C	1151	SER	2.6
2	E	1243	PRO	2.6
2	D	1273	VAL	2.6
1	A	178	VAL	2.5
2	D	1241	ALA	2.5
2	C	1291	SER	2.5
2	C	1145	PHE	2.5
2	C	1194	MET	2.5
1	B	125	HIS	2.5
2	C	1267	ILE	2.5
2	D	1306	TRP	2.4
2	C	1189	TYR	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	1328	ILE	2.4
2	D	1316	LEU	2.4
2	E	1169	SER	2.4
1	B	121	ARG	2.4
2	E	1138	ALA	2.4
2	E	1342	ASP	2.4
2	C	1128	GLY	2.4
1	B	178	VAL	2.4
2	E	1242	GLU	2.3
2	D	1270	MET	2.3
2	C	1150	PRO	2.3
2	E	1216	HIS	2.3
2	D	1249	GLU	2.3
2	C	1135	ALA	2.3
1	B	245	ASN	2.3
2	E	1293	PRO	2.2
1	A	64	ALA	2.2
2	C	1230	VAL	2.2
2	C	1328	ILE	2.2
2	D	1285	ILE	2.2
1	B	117	ARG	2.2
2	E	1171	ALA	2.2
2	E	1300	ALA	2.2
2	C	1202	GLN	2.2
2	D	1210	LEU	2.2
2	D	1257	TYR	2.2
2	C	1156	GLY	2.2
2	D	1252	ALA	2.2
2	C	1157	TYR	2.2
2	E	1283	LEU	2.2
2	E	1218	GLU	2.1
2	E	1250	ILE	2.1
2	C	1210	LEU	2.1
2	C	1178	VAL	2.1
2	C	1198	ALA	2.1
1	B	158	LYS	2.1
2	D	1238	LEU	2.1
2	D	1250	ILE	2.1
2	E	1290	GLU	2.1
2	E	1259	LEU	2.1
2	D	1267	ILE	2.1
2	C	1160	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	94	TYR	2.0
2	E	1247	ASN	2.0
2	C	1177	LYS	2.0
1	B	146	ASN	2.0
2	C	1231	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	A	294	4/4	0.81	0.33	46,57,63,91	0
3	EDO	B	294	4/4	0.87	0.17	60,69,78,80	0
4	PEG	B	295	7/7	0.92	0.15	53,74,87,89	0
5	CA	D	101	1/1	0.98	0.27	43,43,43,43	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.