



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 07:30 PM EDT

PDB ID : 3DI2  
Title : Crystal structure of the complex of human interleukin-7 with unglycosylated human interleukin-7 receptor alpha ectodomain  
Authors : McElroy, C.A.; Dohm, J.A.; Walsh, S.T.R.  
Deposited on : 2008-06-19  
Resolution : 2.70 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.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

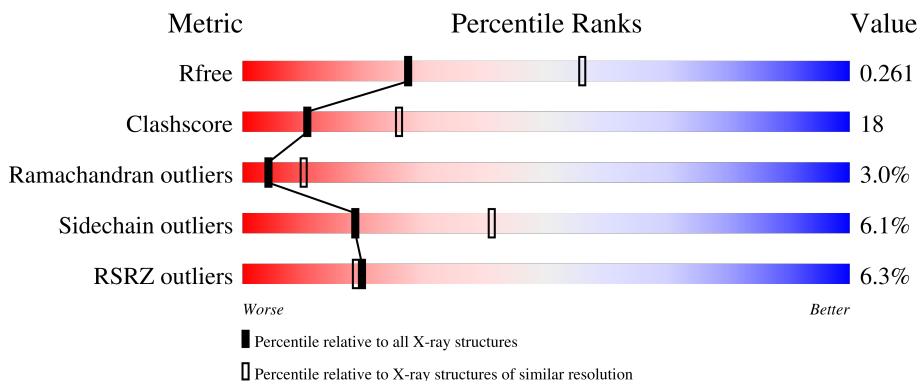
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	154	 3% (poor fit), 41% (0 outliers), 31% (1 outlier), 25% (2+ outliers or not modelled)
1	C	154	 8% (poor fit), 37% (0 outliers), 32% (1 outlier), 29% (2+ outliers or not modelled)
2	B	223	 3% (poor fit), 61% (0 outliers), 24% (1 outlier), 13% (2+ outliers or not modelled)
2	D	223	 7% (poor fit), 52% (0 outliers), 33% (1 outlier), 12% (2+ outliers or not modelled)

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4818 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 Interleukin-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	115	877	561	149	160	7	0	0	0
1	C	110	814	524	135	149	6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P13232
A	0	GLY	-	expression tag	UNP P13232
A	106	ALA	GLU	engineered mutation	UNP P13232
C	-1	MET	-	expression tag	UNP P13232
C	0	GLY	-	expression tag	UNP P13232
C	106	ALA	GLU	engineered mutation	UNP P13232

- Molecule 2 is a protein called Interleukin-7 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	195	1561	1012	253	288	8	0	0	0
2	D	196	1522	985	248	282	7	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

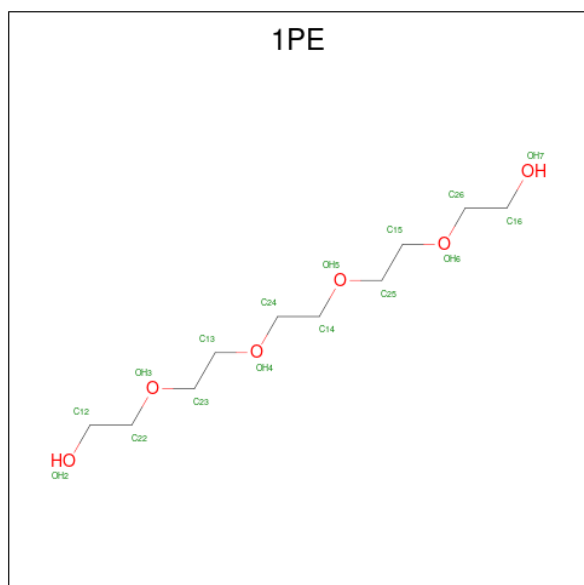
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P16871
B	-2	SER	-	expression tag	UNP P16871
B	-1	HIS	-	expression tag	UNP P16871
B	0	MET	-	expression tag	UNP P16871
B	118	VAL	ILE	engineered mutation	UNP P16871
D	-3	GLY	-	expression tag	UNP P16871

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP P16871
D	-1	HIS	-	expression tag	UNP P16871
D	0	MET	-	expression tag	UNP P16871
D	118	VAL	ILE	engineered mutation	UNP P16871

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
3	A	1	16	10 6	0	0

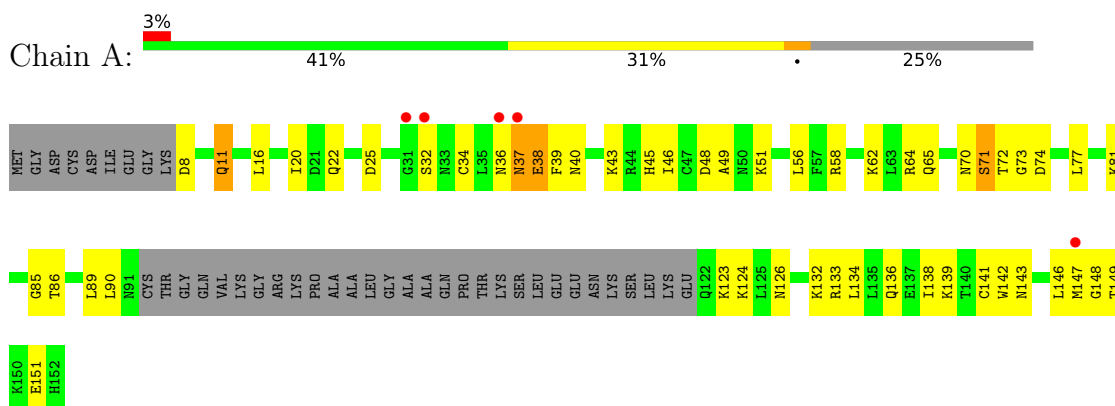
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	14	Total O 14 14	0	0
4	C	1	Total O 1 1	0	0
4	D	4	Total O 4 4	0	0

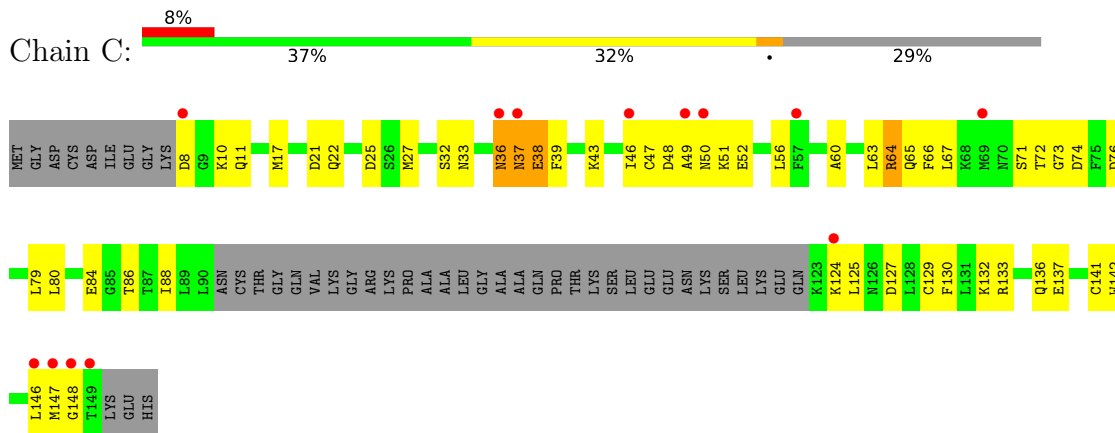
### 3 Residue-property plots [i](#)

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: Interleukin-7

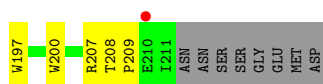


- Molecule 1: Interleukin-7

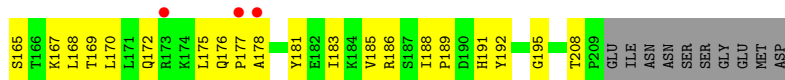
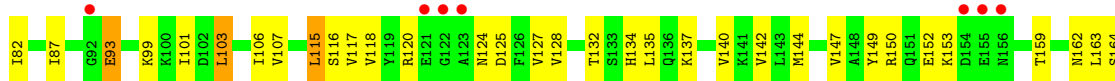


- Molecule 2: Interleukin-7 receptor subunit alpha





- Molecule 2: Interleukin-7 receptor subunit alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.20Å 113.02Å 87.53Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 14.81 – 3.00	Depositor EDS
% Data completeness (in resolution range)	69.6 (15.00-2.70) 96.5 (14.81-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.92 (at 3.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.212 , 0.267 0.209 , 0.261	Depositor DCC
$R_{free}$ test set	1345 reflections (7.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.0	Xtrriage
Anisotropy	0.196	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.096 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: 1PE

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	0.57	0/888	0.63	0/1190
1	C	0.59	1/825 (0.1%)	0.63	0/1112
2	B	0.50	1/1600 (0.1%)	0.71	0/2170
2	D	0.52	1/1559 (0.1%)	0.68	0/2122
All	All	0.53	3/4872 (0.1%)	0.68	0/6594

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	38	GLU	CB-CG	-5.37	1.42	1.52
2	D	93	GLU	CB-CG	-5.25	1.42	1.52
2	B	93	GLU	CB-CG	-5.15	1.42	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	877	0	827	32	0
1	C	814	0	743	41	0
2	B	1561	0	1504	40	0
2	D	1522	0	1429	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	0	22	1	0
4	A	9	0	0	0	0
4	B	14	0	0	1	0
4	C	1	0	0	0	0
4	D	4	0	0	0	0
All	All	4818	0	4525	171	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 18.

All (171) 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:A:38:GLU:HG3	1:A:133:ARG:HH12	1.35	0.88
2:D:80:LEU:HD23	2:D:82:ILE:HB	1.53	0.87
2:D:149:TYR:HB3	2:D:183:ILE:HG13	1.60	0.82
1:C:84:GLU:O	1:C:88:ILE:HG12	1.80	0.80
2:D:118:VAL:HB	2:D:127:VAL:HG13	1.68	0.76
2:D:59:GLU:HB3	2:D:78:LYS:HD3	1.69	0.74
2:B:18:TYR:HE2	2:B:49:LEU:HD11	1.54	0.73
2:B:207:ARG:HD3	4:B:234:HOH:O	1.89	0.72
1:C:64:ARG:HG2	1:C:67:LEU:HD12	1.71	0.72
1:C:38:GLU:CG	1:C:133:ARG:HH12	2.04	0.70
2:B:68:LEU:O	2:B:69:GLN:HB2	1.90	0.70
2:D:80:LEU:CD2	2:D:82:ILE:HB	2.22	0.69
1:C:64:ARG:HB2	1:C:64:ARG:NH1	2.08	0.69
1:A:149:THR:C	1:A:151:GLU:H	1.96	0.68
2:D:41:ASP:HB3	2:D:44:VAL:HG23	1.76	0.68
2:D:175:LEU:HB3	2:D:181:TYR:HE1	1.60	0.66
2:D:117:VAL:HG22	2:D:128:VAL:HG22	1.78	0.66
2:D:118:VAL:HB	2:D:127:VAL:CG1	2.26	0.66
2:B:147:VAL:HG22	2:B:185:VAL:CG1	2.27	0.65
2:B:152:GLU:HG3	2:B:180:MET:O	1.97	0.64
1:A:146:LEU:C	1:A:148:GLY:H	2.02	0.63
2:B:87:ILE:HD12	2:B:101:ILE:HD12	1.79	0.63
2:D:124:ASN:O	2:D:172:GLN:CG	2.48	0.62
2:B:163:LEU:HD22	2:B:168:LEU:HB2	1.82	0.62
1:C:56:LEU:HD21	1:C:141:CYS:HB3	1.82	0.62
1:C:65:GLN:HB3	1:C:125:LEU:HG	1.82	0.62
1:C:64:ARG:HG2	1:C:67:LEU:CD1	2.30	0.60
1:C:66:PHE:HZ	1:C:130:PHE:HD2	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LEU:HD22	1:C:79:LEU:HD22	1.84	0.60
2:D:68:LEU:O	2:D:69:GLN:HB2	2.00	0.60
1:C:8:ASP:C	1:C:10:LYS:H	2.05	0.59
1:A:89:LEU:HD11	2:B:82:ILE:HG21	1.83	0.59
2:B:172:GLN:NE2	2:B:209:PRO:HG2	2.18	0.59
2:B:163:LEU:HD21	2:B:167:LYS:O	2.03	0.59
2:D:188:ILE:HG13	2:D:189:PRO:HD2	1.85	0.59
1:C:72:THR:O	1:C:72:THR:HG23	2.03	0.59
1:A:142:TRP:O	1:A:146:LEU:HG	2.03	0.58
1:C:146:LEU:C	1:C:148:GLY:H	2.07	0.58
2:D:58:VAL:HG23	2:D:59:GLU:H	1.70	0.57
1:A:77:LEU:O	1:A:81:LYS:HG3	2.03	0.57
2:B:152:GLU:HG2	2:B:180:MET:HB3	1.87	0.56
2:D:46:THR:O	2:D:67:LYS:HE2	2.06	0.56
2:B:117:VAL:HG22	2:B:128:VAL:HG22	1.88	0.56
1:C:38:GLU:O	1:C:43:LYS:HE3	2.05	0.55
1:C:17:MET:HG2	1:C:21:ASP:OD2	2.07	0.55
2:D:163:LEU:HG	2:D:165:SER:H	1.70	0.55
1:A:40:ASN:HA	1:A:43:LYS:HG3	1.89	0.55
2:B:168:LEU:HD12	2:B:169:THR:H	1.71	0.55
2:D:20:PHE:CE1	2:D:99:LYS:HD3	2.41	0.55
2:D:134:HIS:HA	2:D:137:LYS:HG3	1.87	0.55
1:C:64:ARG:NH1	1:C:64:ARG:CB	2.69	0.55
1:C:64:ARG:CB	1:C:64:ARG:HH11	2.20	0.55
1:A:132:LYS:O	1:A:136:GLN:HG3	2.07	0.54
2:D:124:ASN:HB3	2:D:172:GLN:CG	2.38	0.54
1:C:8:ASP:C	1:C:10:LYS:N	2.60	0.54
1:C:86:THR:HG23	1:C:142:TRP:HZ2	1.72	0.54
1:A:8:ASP:O	1:A:11:GLN:HB2	2.08	0.54
1:C:66:PHE:CE1	1:C:125:LEU:HD12	2.43	0.54
2:B:168:LEU:HD12	2:B:169:THR:N	2.23	0.53
1:C:46:ILE:HG22	1:C:47:CYS:N	2.24	0.53
2:D:101:ILE:HG21	2:D:106:ILE:HD13	1.91	0.53
2:D:175:LEU:HD22	2:D:181:TYR:CE1	2.44	0.53
1:A:85:GLY:O	1:A:89:LEU:HD13	2.08	0.53
2:D:65:PHE:HA	2:D:74:ILE:HG22	1.90	0.53
1:A:11:GLN:HB3	1:A:89:LEU:HD21	1.90	0.53
1:C:50:ASN:N	1:C:52:GLU:OE2	2.40	0.52
1:A:146:LEU:O	1:A:148:GLY:N	2.41	0.52
2:D:68:LEU:O	2:D:68:LEU:HG	2.09	0.52
2:D:51:PHE:HD2	2:D:72:TYR:CD2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:ALA:HA	2:B:208:THR:O	2.09	0.52
1:C:39:PHE:HD1	1:C:39:PHE:H	1.57	0.52
2:D:35:LEU:HD22	2:D:103:LEU:HD21	1.91	0.51
2:B:132:THR:O	2:B:132:THR:HG23	2.11	0.51
2:B:18:TYR:CE2	2:B:49:LEU:HD11	2.40	0.51
2:B:107:VAL:O	2:B:195:GLY:HA3	2.11	0.51
2:B:149:TYR:HB3	2:B:183:ILE:HG13	1.93	0.51
2:D:115:LEU:HD22	2:D:116:SER:N	2.25	0.51
1:A:149:THR:C	1:A:151:GLU:N	2.63	0.50
1:A:134:LEU:O	1:A:138:ILE:HG13	2.12	0.50
1:C:60:ALA:O	1:C:63:LEU:HB2	2.12	0.50
1:C:39:PHE:CD1	1:C:39:PHE:N	2.79	0.50
2:D:115:LEU:HD22	2:D:116:SER:H	1.76	0.50
2:D:142:VAL:HB	2:D:191:HIS:HB2	1.93	0.50
2:B:188:ILE:HB	2:B:197:TRP:CE3	2.47	0.50
1:C:124:LYS:C	1:C:125:LEU:HD23	2.33	0.49
1:C:86:THR:HG23	1:C:142:TRP:CZ2	2.48	0.49
2:B:73:PHE:CD2	2:B:73:PHE:C	2.86	0.49
2:B:58:VAL:HG23	2:B:59:GLU:H	1.77	0.49
2:D:188:ILE:HG13	2:D:189:PRO:CD	2.42	0.49
2:D:163:LEU:HD21	2:D:167:LYS:O	2.12	0.48
2:B:41:ASP:OD2	2:B:44:VAL:HG23	2.12	0.48
1:A:36:ASN:O	1:A:37:ASN:C	2.52	0.48
1:A:71:SER:O	2:B:59:GLU:HG3	2.13	0.48
2:B:109:PRO:HD3	2:B:189:PRO:HD3	1.96	0.48
2:D:144:MET:O	2:D:188:ILE:HG22	2.13	0.48
2:D:14:GLU:C	2:D:16:ASP:H	2.17	0.48
2:D:115:LEU:CD2	2:D:116:SER:H	2.27	0.47
2:B:125:ASP:OD1	2:B:125:ASP:C	2.53	0.47
1:A:39:PHE:N	1:A:39:PHE:CD1	2.82	0.47
1:A:37:ASN:O	1:A:38:GLU:C	2.52	0.47
1:A:46:ILE:HD12	1:A:46:ILE:N	2.29	0.47
2:D:185:VAL:HG12	2:D:186:ARG:H	1.79	0.47
2:B:147:VAL:HG11	2:B:168:LEU:HD23	1.97	0.47
1:A:62:LYS:HD2	1:A:65:GLN:OE1	2.15	0.47
1:C:146:LEU:O	1:C:148:GLY:N	2.47	0.46
2:D:107:VAL:O	2:D:195:GLY:HA3	2.15	0.46
1:A:123:LYS:HG2	1:A:124:LYS:N	2.30	0.46
1:A:146:LEU:C	1:A:148:GLY:N	2.69	0.46
1:C:88:ILE:HD13	1:C:88:ILE:N	2.31	0.46
1:A:45:HIS:CD2	1:A:58:ARG:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ASP:O	1:C:10:LYS:N	2.49	0.46
1:A:73:GLY:O	1:A:74:ASP:C	2.54	0.46
2:D:150:ARG:O	2:D:181:TYR:HD2	1.98	0.46
1:A:20:ILE:HG21	1:A:139:LYS:HG3	1.96	0.46
1:C:124:LYS:O	1:C:125:LEU:HD23	2.15	0.45
2:D:68:LEU:O	2:D:69:GLN:CB	2.65	0.45
2:D:120:ARG:NH2	2:D:125:ASP:OD2	2.49	0.45
2:D:152:GLU:HG3	2:D:153:LYS:H	1.81	0.45
1:C:73:GLY:O	1:C:74:ASP:C	2.54	0.45
2:D:50:GLU:OE1	2:D:50:GLU:HA	2.16	0.45
2:D:72:TYR:CD1	2:D:72:TYR:N	2.85	0.45
1:A:8:ASP:N	3:A:340:1PE:H122	2.31	0.45
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.78	0.45
2:B:57:LEU:HD13	2:B:63:LEU:HG	1.98	0.45
2:B:50:GLU:HA	2:B:50:GLU:OE1	2.17	0.45
2:B:107:VAL:HG11	2:B:140:VAL:HG21	2.00	0.45
1:A:56:LEU:HD21	1:A:141:CYS:HB3	1.99	0.44
1:C:132:LYS:O	1:C:136:GLN:HG3	2.17	0.44
2:D:191:HIS:CG	2:D:192:TYR:N	2.82	0.44
1:A:48:ASP:O	1:A:49:ALA:C	2.55	0.44
1:C:127:ASP:OD2	1:C:129:CYS:HB2	2.17	0.44
2:D:118:VAL:O	2:D:127:VAL:HG12	2.17	0.44
1:A:70:ASN:O	1:A:72:THR:N	2.46	0.44
1:C:8:ASP:O	1:C:11:GLN:HG3	2.17	0.44
2:B:56:ALA:HB3	2:B:85:SER:OG	2.18	0.44
2:B:176:GLN:HA	2:B:177:PRO:HD3	1.85	0.44
2:D:38:ALA:HB2	2:D:71:ILE:HG22	2.00	0.44
1:C:64:ARG:HB2	1:C:64:ARG:CZ	2.47	0.43
2:D:58:VAL:CG1	2:D:80:LEU:HD12	2.48	0.43
1:C:36:ASN:O	1:C:37:ASN:C	2.57	0.43
1:C:48:ASP:O	1:C:49:ALA:C	2.56	0.43
2:D:87:ILE:HD13	2:D:101:ILE:HD12	2.01	0.43
2:D:147:VAL:HG11	2:D:168:LEU:HD23	2.01	0.42
2:D:132:THR:HG23	2:D:135:LEU:HG	2.00	0.42
2:D:20:PHE:CZ	2:D:99:LYS:HD3	2.54	0.42
2:D:22:CYS:HA	2:D:36:THR:O	2.20	0.42
2:D:65:PHE:HA	2:D:74:ILE:CG2	2.49	0.42
1:A:86:THR:O	1:A:90:LEU:HG	2.19	0.42
2:B:18:TYR:HE2	2:B:49:LEU:CD1	2.30	0.42
2:B:125:ASP:OD1	2:B:125:ASP:O	2.38	0.42
1:C:146:LEU:C	1:C:148:GLY:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:VAL:HG11	2:D:140:VAL:HG21	2.01	0.42
2:D:176:GLN:HA	2:D:177:PRO:HD3	1.81	0.42
2:B:68:LEU:O	2:B:69:GLN:CB	2.63	0.42
1:A:38:GLU:HG3	1:A:133:ARG:NH1	2.18	0.42
2:D:163:LEU:HG	2:D:165:SER:O	2.20	0.41
2:B:138:LYS:HE2	2:B:138:LYS:HA	2.02	0.41
2:D:14:GLU:O	2:D:16:ASP:N	2.49	0.41
2:D:152:GLU:HG3	2:D:153:LYS:N	2.34	0.41
2:D:178:ALA:HA	2:D:208:THR:O	2.19	0.41
1:C:27:MET:CE	1:C:132:LYS:HA	2.50	0.41
2:B:184:LYS:HG3	2:B:200:TRP:CE3	2.56	0.41
2:D:132:THR:HG23	2:D:132:THR:O	2.21	0.41
2:D:149:TYR:OH	2:D:159:THR:HG21	2.20	0.41
2:D:170:LEU:HD22	2:D:170:LEU:N	2.36	0.41
1:A:64:ARG:HB3	1:A:64:ARG:NH1	2.36	0.41
2:B:171:LEU:HD12	2:B:174:LYS:HD2	2.02	0.41
2:B:39:PHE:CZ	2:B:49:LEU:HD13	2.57	0.40
2:D:163:LEU:HD12	2:D:164:SER:H	1.85	0.40
2:B:152:GLU:HG2	2:B:180:MET:CB	2.49	0.40
1:C:79:LEU:HD23	1:C:79:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	111/154 (72%)	91 (82%)	14 (13%)	6 (5%)	<a href="#">2</a> <a href="#">3</a>
1	C	106/154 (69%)	87 (82%)	13 (12%)	6 (6%)	<a href="#">1</a> <a href="#">2</a>
2	B	193/223 (86%)	174 (90%)	17 (9%)	2 (1%)	<a href="#">15</a> <a href="#">37</a>
2	D	194/223 (87%)	175 (90%)	15 (8%)	4 (2%)	<a href="#">7</a> <a href="#">18</a>
All	All	604/754 (80%)	527 (87%)	59 (10%)	18 (3%)	<a href="#">4</a> <a href="#">10</a>

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	C	51	LYS
1	A	147	MET
2	B	69	GLN
2	B	103	LEU
1	C	147	MET
2	D	15	LEU
2	D	69	GLN
2	D	103	LEU
1	A	32	SER
1	A	37	ASN
1	A	71	SER
1	C	32	SER
1	A	38	GLU
1	C	37	ASN
1	C	71	SER
1	C	33	ASN
2	D	93	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	86/136 (63%)	79 (92%)	7 (8%)	11	27
1	C	77/136 (57%)	71 (92%)	6 (8%)	12	29
2	B	169/204 (83%)	159 (94%)	10 (6%)	19	43
2	D	158/204 (78%)	151 (96%)	7 (4%)	28	56
All	All	490/680 (72%)	460 (94%)	30 (6%)	18	41

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	16	LEU

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Mol	Chain	Res	Type
1	A	22	GLN
1	A	25	ASP
1	A	34	CYS
1	A	126	ASN
1	A	143	ASN
2	B	45	ASN
2	B	47	THR
2	B	59	GLU
2	B	73	PHE
2	B	115	LEU
2	B	131	ASN
2	B	136	GLN
2	B	152	GLU
2	B	170	LEU
2	B	185	VAL
1	C	22	GLN
1	C	25	ASP
1	C	36	ASN
1	C	64	ARG
1	C	76	ASP
1	C	137	GLU
2	D	17	ASP
2	D	34	SER
2	D	72	TYR
2	D	80	LEU
2	D	115	LEU
2	D	162	ASN
2	D	169	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	45	ASN
2	B	151	GLN
2	D	191	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	1PE	A	340	-	15,15,15	0.63	0	14,14,14	0.79	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	1PE	A	340	-	-	4/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	340	1PE	OH5-C14-C24-OH4
3	A	340	1PE	OH4-C13-C23-OH3
3	A	340	1PE	OH7-C16-C26-OH6
3	A	340	1PE	OH6-C15-C25-OH5



There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	340	1PE	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	115/154 (74%)	0.04	5 (4%) 35 33	25, 44, 74, 83	0
1	C	110/154 (71%)	0.31	13 (11%) 4 3	25, 49, 73, 85	0
2	B	195/223 (87%)	-0.01	6 (3%) 49 49	19, 40, 67, 84	2 (1%)
2	D	196/223 (87%)	0.16	15 (7%) 13 11	22, 47, 73, 86	1 (0%)
All	All	616/754 (81%)	0.11	39 (6%) 20 19	19, 45, 73, 86	3 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	156	ASN	6.3
1	C	149	THR	5.2
1	C	69	MET	4.3
2	D	154	ASP	3.9
1	C	49	ALA	3.8
2	D	178	ALA	3.8
2	D	156	ASN	3.8
2	D	177	PRO	3.5
2	D	121	GLU	3.4
2	D	122	GLY	3.4
2	B	155	GLU	3.1
1	A	31	GLY	3.0
1	C	148	GLY	3.0
2	D	17	ASP	2.9
1	A	147	MET	2.8
2	D	15	LEU	2.8
1	C	36	ASN	2.8
2	D	155	GLU	2.6
1	C	37	ASN	2.6
1	C	57	PHE	2.5
2	D	16	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	147	MET	2.5
2	B	121	GLU	2.5
1	A	32	SER	2.5
2	B	154	ASP	2.4
2	D	92	GLY	2.4
1	C	146	LEU	2.3
2	D	14	GLU	2.3
2	D	173	ARG	2.3
2	D	123	ALA	2.3
1	A	37	ASN	2.2
1	C	50	ASN	2.2
2	B	210	GLU	2.2
1	C	46	ILE	2.2
1	C	8	ASP	2.1
1	C	124	LYS	2.1
2	D	47	THR	2.1
2	B	91	VAL	2.1
1	A	36	ASN	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	1PE	A	340	16/16	0.69	0.28	66,71,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.