



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 09:20 AM EST

PDB ID : 1C3H
Title : ACRP30 CALCIUM COMPLEX
Authors : Shapiro, L.; Boggon, T.; Scherer, P.
Deposited on : 1999-07-27
Resolution : 2.10 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 : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

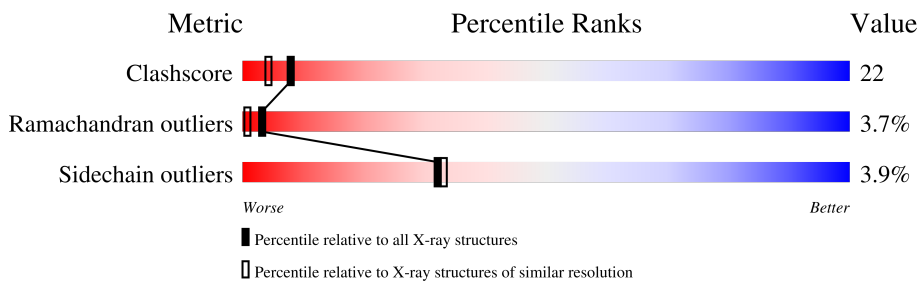
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	137	55% 39% 5% .
1	B	137	69% 26% . .
1	C	137	62% 31% 6% .
1	D	137	62% 35% . .
1	E	137	64% 33% .
1	F	137	65% 32% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7182 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 30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	137	1099	711	177	208	3	0	0	0
1	B	137	1106	715	179	209	3	0	0	0
1	C	137	1098	710	178	207	3	0	0	0
1	D	137	1124	727	181	213	3	0	0	0
1	E	137	1124	727	181	213	3	0	0	0
1	F	137	1120	724	180	213	3	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Ca 1	0	0
2	E	1	Total 1	Ca 1	0	0
2	F	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total 89	O 89	0	0
3	B	77	Total 77	O 77	0	0
3	C	83	Total 83	O 83	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	85	Total 85	O 85	0	0
3	E	79	Total 79	O 79	0	0
3	F	95	Total 95	O 95	0	0

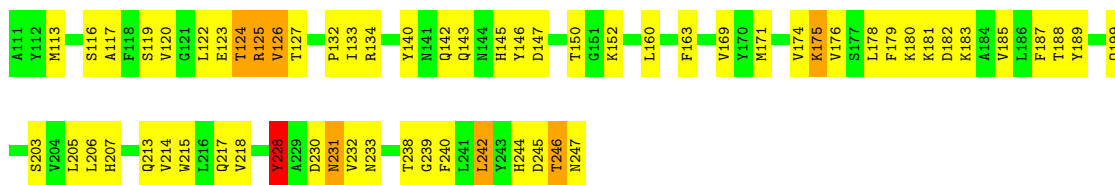
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

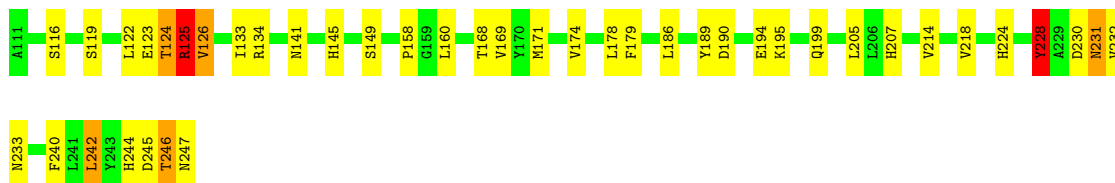
- Molecule 1: 30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR

Chain A: 



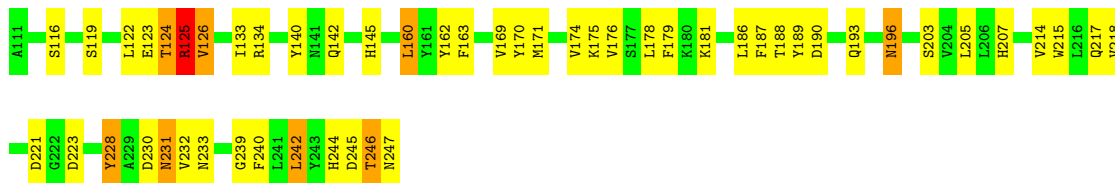
- Molecule 1: 30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR

Chain B: 



- Molecule 1: 30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR

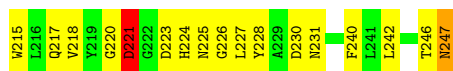
Chain C: 



- Molecule 1: 30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR

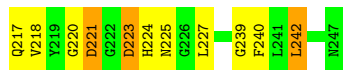
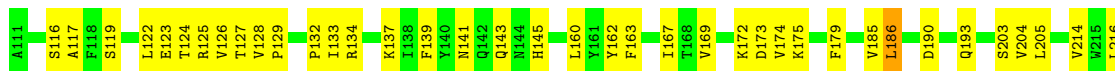
Chain D: 





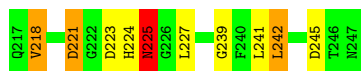
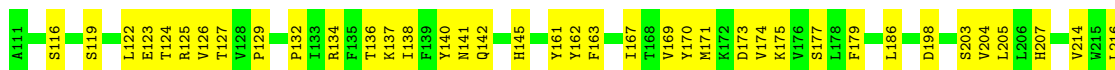
• Molecule 1: 30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR

Chain E: 64% 33%



• Molecule 1: 30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR

Chain F: 65% 32%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.64Å 58.71Å 87.31Å 70.55° 70.62° 60.14°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	93.9 (20.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7182	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

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: 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	0.37	0/1130	0.63	0/1537
1	B	0.36	0/1137	0.62	0/1545
1	C	0.37	0/1129	0.63	0/1536
1	D	0.36	0/1156	0.65	0/1569
1	E	0.36	0/1156	0.66	0/1569
1	F	0.36	0/1152	0.68	0/1565
All	All	0.36	0/6860	0.65	0/9321

There are no bond length outliers.

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	1099	0	1018	55	0
1	B	1106	0	1033	38	0
1	C	1098	0	1018	61	0
1	D	1124	0	1059	53	0
1	E	1124	0	1059	45	0
1	F	1120	0	1048	50	0
2	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	89	0	0	5	0
3	B	77	0	0	0	0
3	C	83	0	0	3	0
3	D	85	0	0	4	0
3	E	79	0	0	3	0
3	F	95	0	0	4	0
All	All	7182	0	6235	278	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 22.

All (278) 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:125:ARG:HH11	1:B:125:ARG:HB3	1.32	0.92
1:F:225:ASN:H	1:F:225:ASN:ND2	1.66	0.92
1:A:125:ARG:HH11	1:A:125:ARG:HB3	1.35	0.91
1:F:225:ASN:H	1:F:225:ASN:HD22	0.91	0.91
1:D:167:ILE:HG21	1:D:227:LEU:HD22	1.53	0.89
1:F:225:ASN:HD22	1:F:225:ASN:N	1.69	0.87
1:F:218:VAL:HG13	1:F:225:ASN:OD1	1.75	0.87
1:B:199:GLN:HE22	1:C:190:ASP:HA	1.40	0.86
1:A:171:MET:HG3	1:A:174:VAL:HG22	1.58	0.85
1:B:244:HIS:CE1	1:B:247:ASN:HD21	1.95	0.84
1:A:244:HIS:CE1	1:A:247:ASN:HD21	1.95	0.83
1:F:174:VAL:HA	1:F:221:ASP:OD2	1.79	0.82
1:A:189:TYR:H	1:C:233:ASN:HD22	1.28	0.82
1:B:171:MET:HG3	1:B:174:VAL:HG22	1.63	0.79
1:C:171:MET:HG3	1:C:174:VAL:HG22	1.68	0.76
1:B:233:ASN:ND2	1:C:189:TYR:H	1.84	0.76
1:A:122:LEU:O	1:A:123:GLU:HB2	1.86	0.76
1:A:199:GLN:HE22	1:B:190:ASP:HA	1.49	0.75
1:D:129:PRO:HA	1:D:218:VAL:CG2	2.15	0.75
1:C:125:ARG:HH22	1:C:134:ARG:HG3	1.51	0.75
1:C:124:THR:O	1:C:125:ARG:HB3	1.87	0.74
1:C:244:HIS:CE1	1:C:247:ASN:HD21	2.05	0.73
1:C:133:ILE:HD11	1:C:218:VAL:HG13	1.71	0.73
1:C:215:TRP:HE1	1:C:217:GLN:HE21	1.35	0.73
1:E:218:VAL:HB	1:E:225:ASN:ND2	2.04	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:PRO:HG3	1:D:224:HIS:HA	1.71	0.72
1:E:175:LYS:N	1:E:221:ASP:HB2	2.04	0.71
1:E:218:VAL:HG22	3:E:1085:HOH:O	1.89	0.71
1:E:218:VAL:HG21	1:E:225:ASN:OD1	1.91	0.71
1:E:167:ILE:HG21	1:E:227:LEU:HD22	1.73	0.71
1:A:189:TYR:H	1:C:233:ASN:ND2	1.89	0.70
1:F:167:ILE:HG21	1:F:227:LEU:HD22	1.74	0.70
1:D:181:LYS:O	1:D:183:LYS:HD3	1.91	0.70
1:F:127:THR:O	1:F:129:PRO:HD3	1.92	0.70
1:D:173:ASP:O	1:D:221:ASP:HB3	1.93	0.69
1:E:129:PRO:HA	1:E:218:VAL:CG2	2.22	0.69
1:B:123:GLU:O	1:B:124:THR:HB	1.93	0.69
1:C:196:ASN:H	1:C:196:ASN:ND2	1.91	0.69
1:C:215:TRP:HE1	1:C:217:GLN:NE2	1.92	0.68
1:E:172:LYS:NZ	1:E:224:HIS:HB3	2.08	0.68
1:B:194:GLU:O	1:B:195:LYS:HB2	1.92	0.68
1:E:218:VAL:HB	1:E:225:ASN:HD21	1.57	0.68
1:F:221:ASP:HB2	1:F:225:ASN:HA	1.74	0.68
1:D:127:THR:HG23	1:D:128:VAL:HG23	1.75	0.68
1:A:123:GLU:O	1:A:124:THR:HB	1.95	0.67
1:B:122:LEU:O	1:B:123:GLU:HB2	1.94	0.67
1:A:124:THR:O	1:A:125:ARG:HB2	1.94	0.67
1:C:246:THR:O	1:C:247:ASN:HB2	1.95	0.67
1:F:173:ASP:O	1:F:221:ASP:HB3	1.94	0.66
1:D:215:TRP:CD1	1:D:217:GLN:HG3	2.31	0.66
1:E:221:ASP:OD2	1:E:225:ASN:HA	1.96	0.66
1:E:172:LYS:HZ1	1:E:224:HIS:HB3	1.61	0.66
1:D:218:VAL:HG22	3:D:1274:HOH:O	1.97	0.65
1:B:233:ASN:HD22	1:C:189:TYR:H	1.44	0.65
1:E:126:VAL:HG21	1:E:227:LEU:HD12	1.80	0.64
1:A:169:VAL:HG12	1:A:171:MET:HG2	1.80	0.64
1:C:125:ARG:C	1:C:125:ARG:HD2	2.18	0.63
1:B:169:VAL:HG12	1:B:171:MET:HG2	1.79	0.63
1:E:175:LYS:H	1:E:221:ASP:HB2	1.63	0.63
1:D:129:PRO:HA	1:D:218:VAL:HG23	1.80	0.63
1:D:134:ARG:NH2	1:D:149:SER:HA	2.14	0.62
1:F:169:VAL:CG2	1:F:198:ASP:HB2	2.29	0.62
1:F:132:PRO:HG2	1:F:134:ARG:NH1	2.14	0.62
1:B:124:THR:O	1:B:125:ARG:HB2	1.99	0.62
1:E:123:GLU:HG3	1:E:137:LYS:HB2	1.81	0.62
1:A:205:LEU:HB2	1:C:119:SER:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG11	1:B:168:THR:O	2.01	0.61
1:D:123:GLU:HG3	1:D:137:LYS:HB2	1.82	0.61
1:C:196:ASN:H	1:C:196:ASN:HD22	1.48	0.61
1:F:123:GLU:HG3	1:F:137:LYS:HB2	1.82	0.60
1:D:186:LEU:HD11	1:D:204:VAL:HB	1.83	0.60
1:D:218:VAL:HB	1:D:221:ASP:OD1	2.02	0.60
1:B:133:ILE:HD11	1:B:218:VAL:HG13	1.83	0.59
1:E:127:THR:HG23	1:E:128:VAL:HG23	1.83	0.59
1:A:240:PHE:CG	1:B:242:LEU:HD11	2.37	0.59
1:C:230:ASP:CG	1:C:231:ASN:H	2.04	0.59
1:D:221:ASP:C	1:D:223:ASP:H	2.06	0.59
1:C:169:VAL:HG12	1:C:171:MET:HG2	1.84	0.59
1:E:169:VAL:HG13	1:E:174:VAL:HG23	1.83	0.58
1:D:247:ASN:HD22	1:D:247:ASN:N	2.01	0.58
1:A:215:TRP:HE1	1:A:217:GLN:NE2	2.02	0.58
1:F:169:VAL:HG21	1:F:198:ASP:HB2	1.85	0.57
1:A:246:THR:O	1:A:247:ASN:HB2	2.04	0.57
1:D:169:VAL:HG13	1:D:174:VAL:HG23	1.86	0.57
1:A:185:VAL:HG11	1:A:206:LEU:HD21	1.85	0.57
1:E:218:VAL:HG11	1:E:225:ASN:CG	2.25	0.56
1:C:196:ASN:HD22	1:C:196:ASN:N	2.02	0.56
1:E:116:SER:OG	1:E:145:HIS:HD2	1.88	0.56
1:B:178:LEU:HB3	1:B:186:LEU:HB2	1.88	0.56
1:B:119:SER:HB2	1:C:205:LEU:HB2	1.86	0.56
1:A:215:TRP:HE1	1:A:217:GLN:HE21	1.54	0.56
1:A:124:THR:HB	1:A:231:ASN:OD1	2.06	0.55
1:C:246:THR:HG22	1:C:247:ASN:N	2.21	0.55
1:D:132:PRO:HD3	1:D:217:GLN:HE21	1.71	0.55
1:E:163:PHE:O	1:E:203:SER:HA	2.07	0.55
1:C:124:THR:HB	1:C:231:ASN:OD1	2.07	0.55
1:C:124:THR:OG1	1:C:231:ASN:ND2	2.40	0.55
1:C:175:LYS:HG2	1:C:189:TYR:CD1	2.42	0.55
1:A:119:SER:HB2	1:B:205:LEU:HB2	1.88	0.54
1:D:240:PHE:CG	1:E:242:LEU:HD11	2.42	0.54
1:D:193:GLN:HG3	1:D:194:GLU:OE1	2.07	0.54
1:A:116:SER:OG	1:A:145:HIS:HD2	1.91	0.54
1:D:205:LEU:HB2	1:F:119:SER:HB2	1.89	0.54
1:D:247:ASN:ND2	1:D:247:ASN:OXT	2.41	0.54
1:C:230:ASP:CG	1:C:231:ASN:N	2.62	0.54
1:A:187:PHE:HD2	1:C:232:VAL:O	1.91	0.53
1:C:126:VAL:HB	3:C:1408:HOH:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LEU:HD13	1:F:140:TYR:CE1	2.44	0.53
1:D:132:PRO:CD	1:D:217:GLN:HE21	2.22	0.53
1:C:125:ARG:NH2	1:C:134:ARG:HG3	2.23	0.53
1:E:119:SER:HB2	1:F:205:LEU:HB2	1.90	0.53
1:E:173:ASP:O	1:E:221:ASP:OD1	2.26	0.53
1:B:123:GLU:O	1:B:124:THR:CB	2.57	0.52
1:B:246:THR:O	1:B:247:ASN:HB2	2.09	0.52
1:F:145:HIS:HE1	3:F:1329:HOH:O	1.90	0.52
1:D:154:TYR:HE1	1:D:213:GLN:NE2	2.08	0.52
1:E:134:ARG:HG2	3:E:1128:HOH:O	2.10	0.52
1:A:189:TYR:N	1:C:233:ASN:HD22	2.03	0.52
1:C:196:ASN:ND2	1:C:196:ASN:N	2.56	0.52
1:D:134:ARG:CZ	1:D:149:SER:HA	2.39	0.52
1:A:182:ASP:OD2	1:A:183:LYS:HG3	2.09	0.51
1:E:119:SER:HB3	1:E:139:PHE:HB2	1.92	0.51
1:F:225:ASN:ND2	1:F:225:ASN:N	2.41	0.51
1:F:218:VAL:HB	3:F:1337:HOH:O	2.10	0.51
1:D:131:VAL:C	1:D:217:GLN:HG2	2.31	0.51
1:D:215:TRP:HE1	1:D:217:GLN:CD	2.14	0.51
1:F:116:SER:OG	1:F:145:HIS:HD2	1.92	0.51
1:C:179:PHE:O	1:C:214:VAL:HA	2.11	0.51
1:E:133:ILE:HG13	1:E:217:GLN:HA	1.92	0.51
1:D:116:SER:OG	1:D:145:HIS:HD2	1.92	0.51
1:B:125:ARG:HB3	1:B:125:ARG:NH1	2.15	0.50
1:F:221:ASP:HB2	1:F:225:ASN:CA	2.41	0.50
1:A:117:ALA:H	1:A:143:GLN:NE2	2.09	0.50
1:A:125:ARG:HB3	1:A:125:ARG:NH1	2.17	0.50
1:C:178:LEU:HB3	1:C:186:LEU:HB3	1.94	0.50
1:E:125:ARG:HB3	3:E:1348:HOH:O	2.10	0.50
1:C:123:GLU:O	1:C:124:THR:HB	2.12	0.49
1:C:190:ASP:O	1:C:193:GLN:HG3	2.12	0.49
1:E:129:PRO:HA	1:E:218:VAL:HG21	1.91	0.49
1:B:126:VAL:HG13	1:B:126:VAL:O	2.12	0.49
1:E:162:TYR:O	1:E:239:GLY:HA2	2.13	0.49
1:C:175:LYS:HG2	1:C:189:TYR:HD1	1.78	0.49
1:D:196:ASN:HB2	1:E:193:GLN:HG3	1.95	0.49
1:E:175:LYS:CG	1:E:220:GLY:H	2.25	0.49
1:A:123:GLU:O	1:A:124:THR:CB	2.61	0.49
1:D:193:GLN:HG3	1:D:194:GLU:CD	2.33	0.49
1:A:132:PRO:HB3	1:A:215:TRP:CD1	2.48	0.49
1:A:231:ASN:OD1	1:A:232:VAL:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ILE:HD11	1:A:218:VAL:HG13	1.94	0.48
1:E:218:VAL:CB	1:E:225:ASN:ND2	2.73	0.48
1:F:161:TYR:CZ	1:F:241:LEU:HD13	2.49	0.48
1:A:207:HIS:HE2	1:A:245:ASP:CG	2.17	0.48
1:C:123:GLU:O	1:C:124:THR:CB	2.61	0.48
1:C:232:VAL:O	1:C:232:VAL:HG12	2.13	0.48
1:D:231:ASN:N	1:D:231:ASN:HD22	2.11	0.48
1:A:125:ARG:HH11	1:A:125:ARG:CB	2.16	0.48
1:D:246:THR:OG1	1:D:247:ASN:N	2.46	0.48
1:A:228:TYR:HA	3:A:1412:HOH:O	2.13	0.48
1:A:180:LYS:HG2	1:A:181:LYS:HG3	1.94	0.48
1:C:116:SER:OG	1:C:145:HIS:HD2	1.96	0.48
1:A:242:LEU:HD11	1:C:240:PHE:CG	2.49	0.47
1:D:128:VAL:HB	1:D:131:VAL:HG21	1.96	0.47
1:A:126:VAL:HB	3:A:1407:HOH:O	2.13	0.47
1:D:119:SER:HB2	1:E:205:LEU:HB2	1.96	0.47
1:F:174:VAL:HA	1:F:221:ASP:CG	2.34	0.47
1:F:175:LYS:H	1:F:221:ASP:CG	2.17	0.47
1:F:221:ASP:C	1:F:223:ASP:H	2.17	0.47
1:A:152:LYS:HD3	1:A:213:GLN:NE2	2.30	0.47
1:F:162:TYR:O	1:F:239:GLY:HA2	2.15	0.47
1:D:132:PRO:HG2	3:D:1279:HOH:O	2.14	0.47
1:D:175:LYS:HG2	1:D:220:GLY:H	1.80	0.47
1:D:230:ASP:HB2	3:D:1500:HOH:O	2.13	0.47
1:F:224:HIS:O	1:F:225:ASN:O	2.33	0.47
1:D:193:GLN:OE1	1:D:193:GLN:HA	2.15	0.47
1:D:221:ASP:C	1:D:223:ASP:N	2.68	0.46
1:F:221:ASP:CG	1:F:225:ASN:HB3	2.36	0.46
1:D:193:GLN:O	1:D:194:GLU:C	2.53	0.46
1:E:174:VAL:HG22	1:E:227:LEU:HD23	1.96	0.46
1:D:129:PRO:O	1:D:131:VAL:HG13	2.16	0.46
1:C:186:LEU:HD13	1:C:187:PHE:N	2.31	0.46
1:F:169:VAL:HG12	1:F:174:VAL:HG21	1.97	0.46
1:C:171:MET:HB2	1:C:221:ASP:O	2.16	0.46
1:E:117:ALA:H	1:E:143:GLN:NE2	2.14	0.46
1:F:170:TYR:CD2	1:F:171:MET:HG2	2.51	0.46
1:C:124:THR:O	1:C:125:ARG:CB	2.61	0.45
1:C:160:LEU:HD21	1:C:205:LEU:HB3	1.98	0.45
1:E:169:VAL:HG21	1:E:190:ASP:HB3	1.98	0.45
1:F:122:LEU:HD21	1:F:126:VAL:HG23	1.98	0.45
1:D:170:TYR:O	1:D:171:MET:HB2	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:HIS:CE1	1:A:247:ASN:ND2	2.74	0.45
1:A:124:THR:OG1	1:A:231:ASN:ND2	2.50	0.45
1:C:230:ASP:O	1:C:231:ASN:HB3	2.16	0.45
1:A:124:THR:O	1:A:125:ARG:CB	2.65	0.45
1:A:233:ASN:ND2	1:B:189:TYR:H	2.15	0.45
1:B:233:ASN:HD22	1:C:189:TYR:N	2.13	0.45
1:E:221:ASP:OD1	1:E:221:ASP:C	2.55	0.45
1:A:179:PHE:O	1:A:214:VAL:HA	2.16	0.45
1:A:125:ARG:O	1:A:127:THR:HG23	2.18	0.44
1:B:116:SER:OG	1:B:145:HIS:HD2	2.00	0.44
1:E:185:VAL:HG23	1:E:186:LEU:N	2.32	0.44
1:C:123:GLU:O	1:C:124:THR:HG22	2.17	0.44
1:E:132:PRO:O	1:E:134:ARG:NE	2.50	0.44
1:F:138:ILE:N	1:F:138:ILE:HD12	2.32	0.44
1:D:127:THR:HG23	1:D:128:VAL:N	2.32	0.44
1:B:126:VAL:CG1	1:B:168:THR:O	2.65	0.44
1:C:207:HIS:NE2	1:C:245:ASP:OD2	2.48	0.44
1:D:132:PRO:HG2	3:D:1268:HOH:O	2.18	0.44
1:E:122:LEU:HD21	1:E:126:VAL:HG23	1.99	0.44
1:B:207:HIS:NE2	1:B:245:ASP:OD2	2.50	0.44
1:F:137:LYS:NZ	3:F:1324:HOH:O	2.51	0.44
1:F:163:PHE:O	1:F:203:SER:HA	2.18	0.44
1:F:179:PHE:O	1:F:214:VAL:HA	2.18	0.44
1:A:140:TYR:CZ	1:A:142:GLN:HB2	2.53	0.44
1:C:244:HIS:CE1	1:C:247:ASN:ND2	2.82	0.43
1:F:175:LYS:N	1:F:221:ASP:OD1	2.46	0.43
1:F:177:SER:HA	1:F:186:LEU:O	2.18	0.43
1:B:244:HIS:CE1	1:B:247:ASN:ND2	2.74	0.43
1:B:134:ARG:HD3	1:B:149:SER:O	2.19	0.43
1:F:207:HIS:HE2	1:F:245:ASP:CG	2.21	0.43
1:A:176:VAL:HB	1:A:188:THR:HB	2.00	0.43
1:B:179:PHE:O	1:B:214:VAL:HA	2.18	0.43
1:C:163:PHE:O	1:C:203:SER:HA	2.18	0.43
1:F:132:PRO:HG2	1:F:134:ARG:HH12	1.83	0.43
1:D:129:PRO:CG	1:D:224:HIS:HA	2.44	0.43
1:A:120:VAL:HG11	1:A:146:TYR:CD2	2.54	0.43
1:A:230:ASP:O	1:A:231:ASN:HB3	2.19	0.43
1:B:125:ARG:HH11	1:B:125:ARG:CB	2.16	0.43
1:A:125:ARG:NH2	3:A:1415:HOH:O	2.52	0.43
1:B:122:LEU:HD21	1:B:134:ARG:O	2.19	0.43
1:E:240:PHE:CG	1:F:242:LEU:HD11	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:GLN:NE2	3:F:1320:HOH:O	2.51	0.43
1:A:213:GLN:NE2	3:A:1375:HOH:O	2.52	0.42
1:F:129:PRO:HA	1:F:218:VAL:CG1	2.49	0.42
1:F:170:TYR:O	1:F:171:MET:HB2	2.19	0.42
1:F:136:THR:O	1:F:138:ILE:CD1	2.68	0.42
1:A:147:ASP:OD2	1:A:150:THR:HG23	2.20	0.42
1:E:127:THR:HG23	1:E:128:VAL:N	2.35	0.42
1:E:221:ASP:OD2	1:E:225:ASN:CA	2.66	0.42
1:A:113:MET:HA	1:A:113:MET:HE2	2.01	0.42
1:B:240:PHE:CG	1:C:242:LEU:HD11	2.55	0.42
1:C:122:LEU:O	1:C:123:GLU:CB	2.68	0.42
1:B:228:TYR:HE2	1:B:231:ASN:HD22	1.68	0.42
1:D:175:LYS:HB3	1:D:220:GLY:C	2.40	0.42
1:C:170:TYR:OH	1:C:231:ASN:ND2	2.53	0.42
1:C:207:HIS:HE2	1:C:245:ASP:CG	2.22	0.42
1:A:178:LEU:C	1:A:178:LEU:HD13	2.40	0.42
1:C:140:TYR:CZ	1:C:142:GLN:HB2	2.55	0.42
1:A:163:PHE:O	1:A:203:SER:HA	2.20	0.42
1:C:162:TYR:O	1:C:239:GLY:HA2	2.20	0.41
1:F:204:VAL:HG22	1:F:205:LEU:N	2.33	0.41
1:D:167:ILE:HD13	1:D:227:LEU:HD22	2.02	0.41
1:A:134:ARG:HD2	3:A:1321:HOH:O	2.21	0.41
1:A:175:LYS:HG3	1:A:189:TYR:CD1	2.55	0.41
1:C:223:ASP:HB3	3:C:1395:HOH:O	2.19	0.41
1:F:124:THR:C	1:F:125:ARG:HD2	2.40	0.41
1:F:221:ASP:OD1	1:F:225:ASN:OD1	2.38	0.41
1:B:230:ASP:O	1:B:231:ASN:CB	2.68	0.41
1:C:231:ASN:OD1	1:C:232:VAL:N	2.53	0.41
1:D:231:ASN:N	1:D:231:ASN:ND2	2.67	0.41
1:A:238:THR:HG22	1:A:239:GLY:N	2.35	0.41
1:B:232:VAL:O	1:B:232:VAL:HG12	2.20	0.41
1:E:221:ASP:O	1:E:223:ASP:N	2.53	0.41
1:D:116:SER:OG	1:D:145:HIS:CD2	2.74	0.41
1:D:163:PHE:O	1:D:203:SER:HA	2.20	0.41
1:A:242:LEU:HD11	1:C:240:PHE:CB	2.51	0.41
1:E:179:PHE:O	1:E:214:VAL:HA	2.20	0.41
1:C:181:LYS:HA	3:C:1033:HOH:O	2.21	0.41
1:B:158:PRO:O	1:B:244:HIS:HD2	2.04	0.40
1:D:175:LYS:HG2	1:D:220:GLY:N	2.35	0.40
1:E:221:ASP:OD2	1:E:225:ASN:ND2	2.48	0.40
1:F:127:THR:O	1:F:127:THR:HG22	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:OG1	1:B:231:ASN:ND2	2.51	0.40
1:C:176:VAL:HB	1:C:188:THR:HB	2.02	0.40
1:D:215:TRP:NE1	1:D:217:GLN:HG3	2.36	0.40
1:E:204:VAL:HG22	1:E:205:LEU:N	2.36	0.40
1:F:169:VAL:O	1:F:169:VAL:HG23	2.22	0.40
1:D:125:ARG:HE	1:D:228:TYR:HD1	1.68	0.40
1:F:221:ASP:CB	1:F:225:ASN:HA	2.49	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	135/137 (98%)	110 (82%)	19 (14%)	6 (4%)	2 0
1	B	135/137 (98%)	111 (82%)	17 (13%)	7 (5%)	2 0
1	C	135/137 (98%)	106 (78%)	23 (17%)	6 (4%)	2 0
1	D	135/137 (98%)	115 (85%)	14 (10%)	6 (4%)	2 0
1	E	135/137 (98%)	117 (87%)	16 (12%)	2 (2%)	10 5
1	F	135/137 (98%)	118 (87%)	14 (10%)	3 (2%)	6 2
All	All	810/822 (98%)	677 (84%)	103 (13%)	30 (4%)	3 1

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	THR
1	A	125	ARG
1	A	126	VAL
1	A	246	THR
1	B	124	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	125	ARG
1	B	228	TYR
1	B	246	THR
1	C	124	THR
1	C	125	ARG
1	C	228	TYR
1	C	246	THR
1	D	194	GLU
1	D	221	ASP
1	F	221	ASP
1	F	225	ASN
1	A	228	TYR
1	B	231	ASN
1	C	126	VAL
1	C	231	ASN
1	D	130	ASN
1	A	231	ASN
1	E	141	ASN
1	D	141	ASN
1	F	141	ASN
1	D	225	ASN
1	B	141	ASN
1	D	226	GLY
1	E	124	THR
1	B	126	VAL

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	116/122 (95%)	112 (97%)	4 (3%)	37	39
1	B	118/122 (97%)	113 (96%)	5 (4%)	30	30
1	C	116/122 (95%)	111 (96%)	5 (4%)	29	29
1	D	122/122 (100%)	118 (97%)	4 (3%)	38	40
1	E	122/122 (100%)	116 (95%)	6 (5%)	25	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	121/122 (99%)	117 (97%)	4 (3%)	38	40
All	All	715/732 (98%)	687 (96%)	28 (4%)	32	33

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	LEU
1	A	175	LYS
1	A	228	TYR
1	A	242	LEU
1	B	125	ARG
1	B	160	LEU
1	B	224	HIS
1	B	228	TYR
1	B	242	LEU
1	C	125	ARG
1	C	160	LEU
1	C	196	ASN
1	C	228	TYR
1	C	242	LEU
1	D	130	ASN
1	D	221	ASP
1	D	242	LEU
1	D	247	ASN
1	E	160	LEU
1	E	186	LEU
1	E	216	LEU
1	E	221	ASP
1	E	223	ASP
1	E	242	LEU
1	F	216	LEU
1	F	218	VAL
1	F	225	ASN
1	F	242	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	145	HIS
1	A	213	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	244	HIS
1	A	247	ASN
1	B	143	GLN
1	B	145	HIS
1	B	196	ASN
1	B	199	GLN
1	B	233	ASN
1	B	244	HIS
1	B	247	ASN
1	C	143	GLN
1	C	145	HIS
1	C	199	GLN
1	C	233	ASN
1	C	244	HIS
1	D	143	GLN
1	D	145	HIS
1	D	199	GLN
1	D	213	GLN
1	D	217	GLN
1	D	231	ASN
1	D	247	ASN
1	E	143	GLN
1	E	145	HIS
1	E	213	GLN
1	F	143	GLN
1	F	145	HIS
1	F	225	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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.