



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:36 AM UTC

PDB ID : 5C5B / pdb_00005c5b
Title : Crystal Structure of Human APPL BAR-PH Heterodimer
Authors : Chen, Y.J.; Chen, B.
Deposited on : 2015-06-19
Resolution : 2.90 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

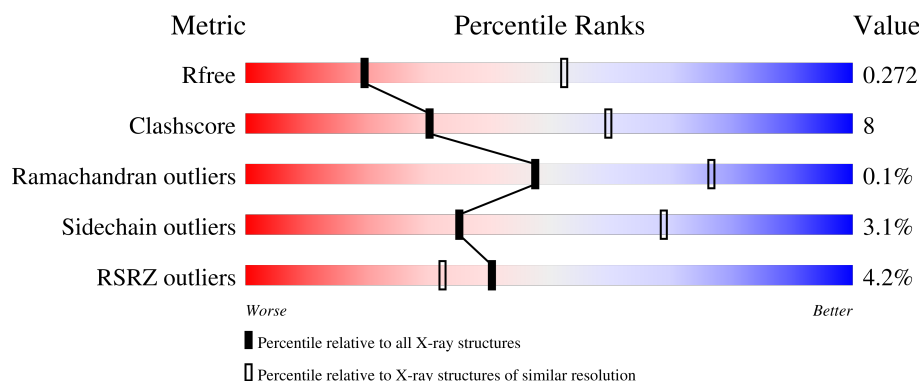
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	375	4% 74% 20% • 5%
1	C	375	4% 76% 17% • 5%
2	B	375	5% 75% 21% ...
2	D	375	3% 82% 16% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11349 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 DCC-interacting protein 13-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2805	1753	475	557	20			
1	C	358	Total	C	N	O	S	0	0	0
			2797	1752	471	554	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9UKG1
A	2	SER	-	expression tag	UNP Q9UKG1
A	3	HIS	-	expression tag	UNP Q9UKG1
A	4	MET	-	expression tag	UNP Q9UKG1
C	1	GLY	-	expression tag	UNP Q9UKG1
C	2	SER	-	expression tag	UNP Q9UKG1
C	3	HIS	-	expression tag	UNP Q9UKG1
C	4	MET	-	expression tag	UNP Q9UKG1

- Molecule 2 is a protein called DCC-interacting protein 13-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	370	Total	C	N	O	S	0	0	0
			2862	1789	484	568	21			
2	D	371	Total	C	N	O	S	0	0	0
			2844	1781	482	560	21			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

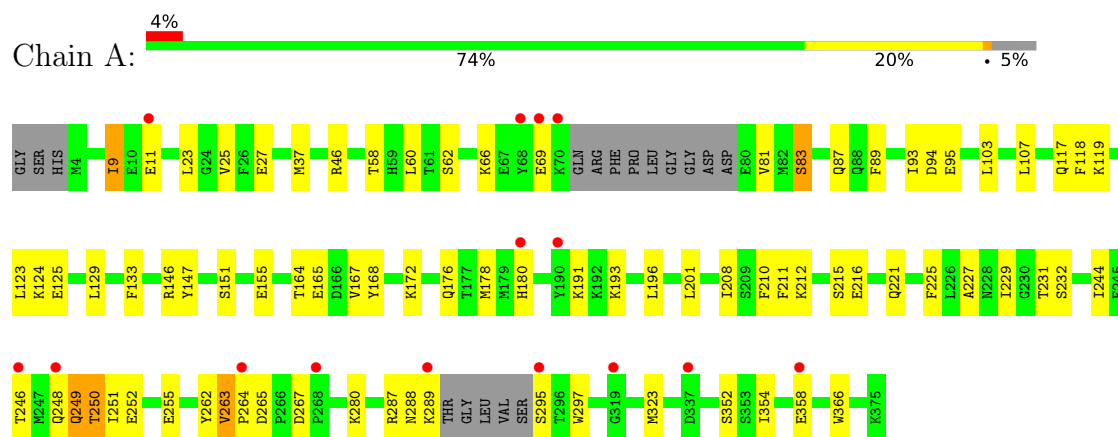
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	6	Total	O	0	0
			6	6		
4	C	6	Total	O	0	0
			6	6		
4	D	6	Total	O	0	0
			6	6		

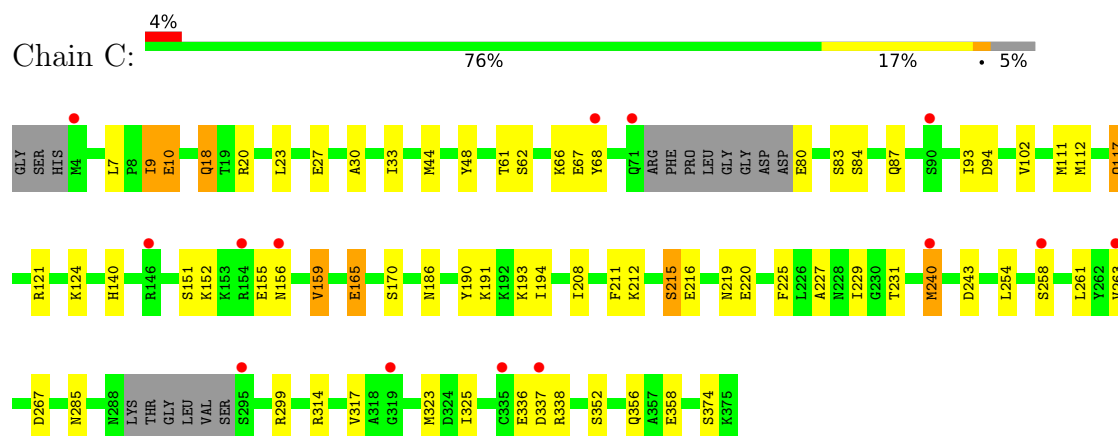
3 Residue-property plots [i](#)

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.

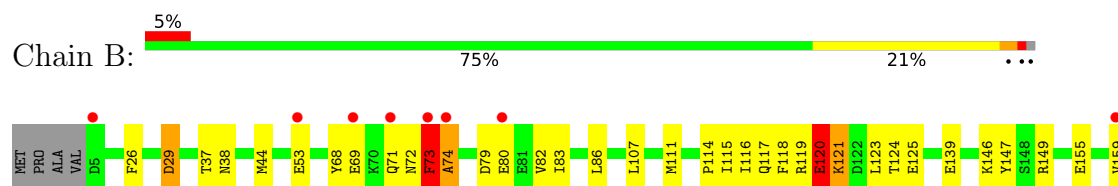
• Molecule 1: DCC-interacting protein 13-alpha

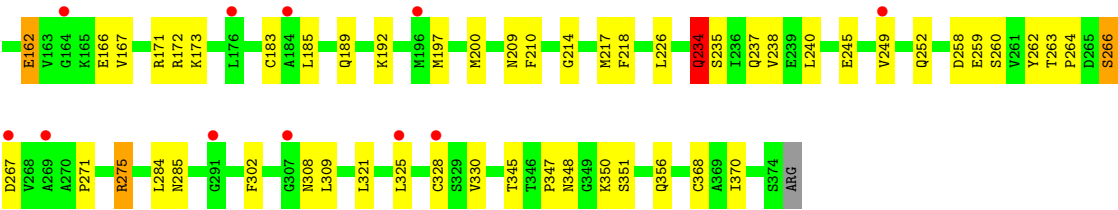


• Molecule 1: DCC-interacting protein 13-alpha

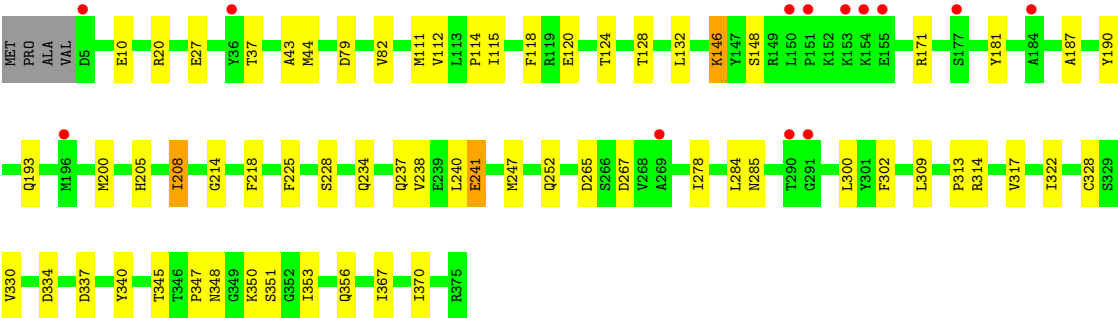
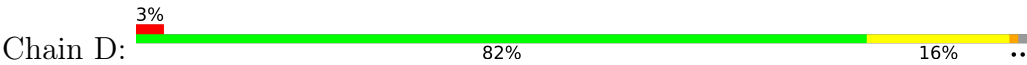


• Molecule 2: DCC-interacting protein 13-beta





● Molecule 2: DCC-interacting protein 13-beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.92Å 88.54Å 147.39Å 90.00° 92.65° 90.00°	Depositor
Resolution (Å)	49.08 – 2.90 49.08 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.08-2.90) 99.0 (49.08-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9-1692	Depositor
R, R_{free}	0.210 , 0.268 0.217 , 0.272	Depositor DCC
R_{free} test set	2389 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	1.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11349	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1008e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
GOL

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	0.36	0/2849	0.82	8/3848 (0.2%)
1	C	0.36	0/2842	0.82	12/3840 (0.3%)
2	B	0.39	0/2903	0.87	5/3927 (0.1%)
2	D	0.32	0/2885	0.77	0/3907
All	All	0.36	0/11479	0.82	25/15522 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	74	ALA	N-CA-C	10.54	122.77	111.28
1	C	215	SER	CA-C-N	-8.16	109.95	123.33
1	C	215	SER	C-N-CA	-8.16	109.95	123.33
1	A	250	THR	N-CA-C	-8.11	102.52	111.36
2	B	234	GLN	CA-CB-CG	-6.21	101.67	114.10
1	C	240	MET	N-CA-C	6.09	120.79	113.23
1	A	216	GLU	N-CA-C	5.71	119.94	112.92
1	C	263	VAL	CA-C-N	5.66	124.85	118.97
1	C	263	VAL	C-N-CA	5.66	124.85	118.97
1	C	7	LEU	CA-C-N	5.64	126.90	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	LEU	C-N-CA	5.64	126.90	119.84
1	C	240	MET	CA-CB-CG	-5.59	102.92	114.10
2	B	120	GLU	CA-C-N	-5.51	112.38	121.92
2	B	120	GLU	C-N-CA	-5.51	112.38	121.92
1	A	267	ASP	CA-C-N	5.51	125.86	119.47
1	A	267	ASP	C-N-CA	5.51	125.86	119.47
2	B	155	GLU	N-CA-C	5.44	117.38	108.52
1	C	240	MET	CA-C-N	-5.40	111.69	121.14
1	C	240	MET	C-N-CA	-5.40	111.69	121.14
1	A	263	VAL	CA-C-N	5.26	124.71	119.24
1	A	263	VAL	C-N-CA	5.26	124.71	119.24
1	C	267	ASP	CA-C-N	5.06	125.33	119.47
1	C	267	ASP	C-N-CA	5.06	125.33	119.47
1	A	66	LYS	CA-C-N	-5.05	114.66	122.49
1	A	66	LYS	C-N-CA	-5.05	114.66	122.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	73	PHE	Peptide
1	C	216	GLU	Peptide

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	2805	0	2687	53	0
1	C	2797	0	2670	56	0
2	B	2862	0	2767	68	0
2	D	2844	0	2734	53	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
3	D	6	0	8	1	0
4	A	5	0	0	0	0
4	B	6	0	0	0	0
4	C	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	6	0	0	0	0
All	All	11349	0	10882	186	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 8.

All (186) 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:D:190:TYR:HA	2:D:193:GLN:HE21	1.35	0.91
2:B:348:ASN:HD21	2:B:350:LYS:HE2	1.36	0.90
2:B:234:GLN:NE2	2:B:237:GLN:OE1	2.05	0.90
1:A:193:LYS:HD2	2:B:82:VAL:HG11	1.65	0.79
1:C:186:ASN:HD22	2:D:247:MET:HE1	1.46	0.79
1:C:208:ILE:HG12	2:D:218:PHE:HB3	1.69	0.75
2:B:267:ASP:HB2	2:B:271:PRO:HA	1.70	0.74
2:B:258:ASP:OD1	2:B:259:GLU:N	2.22	0.72
1:A:62:SER:OG	1:A:94:ASP:OD2	2.07	0.71
2:B:121:LYS:O	2:B:125:GLU:HB2	1.88	0.71
1:C:48:TYR:HB2	1:C:112:MET:HE3	1.72	0.71
1:A:83:SER:O	1:A:87:GLN:HG3	1.91	0.69
1:A:208:ILE:HG12	2:B:218:PHE:HB3	1.74	0.69
1:C:61:THR:HG22	2:D:43:ALA:HB1	1.74	0.68
1:A:119:LYS:HD2	1:A:123:LEU:HD12	1.75	0.67
2:D:146:LYS:HD3	3:D:401:GOL:H32	1.77	0.67
2:B:80:GLU:HA	2:B:83:ILE:HB	1.78	0.65
1:A:229:ILE:HG23	2:B:197:MET:HE2	1.77	0.65
2:B:263:THR:O	2:B:266:SER:OG	2.16	0.63
1:A:232:SER:HB2	2:B:197:MET:HE1	1.80	0.63
1:C:225:PHE:HZ	2:D:200:MET:HB3	1.63	0.63
1:C:240:MET:CE	2:D:187:ALA:HA	2.29	0.63
2:B:260:SER:HB2	2:B:266:SER:HB3	1.80	0.62
2:B:348:ASN:ND2	2:B:350:LYS:HE2	2.11	0.62
2:B:69:GLU:HG3	2:B:83:ILE:HG12	1.81	0.62
1:C:258:SER:HA	1:C:261:LEU:HD12	1.81	0.62
1:A:323:MET:HG3	1:A:352:SER:HB3	1.83	0.61
2:D:267:ASP:OD1	2:D:267:ASP:N	2.33	0.61
1:C:240:MET:HE2	2:D:187:ALA:HA	1.84	0.60
2:B:345:THR:HG22	2:B:351:SER:HA	1.84	0.59
1:A:358:GLU:OE2	2:B:171:ARG:NH2	2.35	0.59
1:C:338:ARG:NH2	2:D:148:SER:OG	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:O	1:A:250:THR:OG1	2.11	0.59
1:A:95:GLU:OE1	1:A:221:GLN:NE2	2.37	0.57
2:B:139:GLU:OE1	2:B:173:LYS:NZ	2.35	0.57
2:D:37:THR:HG21	2:D:118:PHE:HE2	1.70	0.57
1:C:156:ASN:ND2	1:C:159:VAL:H	2.03	0.57
1:C:323:MET:HG3	1:C:352:SER:HB3	1.86	0.56
2:B:234:GLN:O	2:B:238:VAL:HG13	2.05	0.56
1:A:176:GLN:O	1:A:180:HIS:ND1	2.28	0.56
1:C:254:LEU:HD21	2:D:10:GLU:HA	1.88	0.56
1:A:196:LEU:HD23	2:B:86:LEU:HD21	1.88	0.56
1:A:248:GLN:O	1:A:251:ILE:HB	2.06	0.56
2:D:120:GLU:O	2:D:124:THR:OG1	2.17	0.56
2:B:328:CYS:SG	2:B:347:PRO:HD3	2.46	0.55
1:A:249:GLN:HA	1:A:252:GLU:H	1.71	0.55
1:C:358:GLU:OE2	2:D:171:ARG:NH2	2.37	0.55
2:B:38:ASN:OD1	2:B:119:ARG:NH1	2.40	0.55
1:C:83:SER:O	1:C:87:GLN:HG3	2.06	0.55
1:A:358:GLU:CD	2:B:171:ARG:HH22	2.15	0.55
1:C:67:GLU:HG3	1:C:68:TYR:CD1	2.42	0.55
1:C:66:LYS:NZ	1:C:94:ASP:OD2	2.41	0.54
1:C:30:ALA:HA	1:C:33:ILE:HD12	1.89	0.54
2:B:120:GLU:O	2:B:124:THR:OG1	2.18	0.53
2:D:285:ASN:HB2	2:D:356:GLN:HB3	1.89	0.53
1:C:18:GLN:NE2	2:D:317:VAL:O	2.40	0.53
1:A:165:GLU:HA	1:A:168:TYR:HB3	1.89	0.53
2:D:79:ASP:HB3	2:D:82:VAL:HG22	1.90	0.53
2:B:114:PRO:HA	2:B:117:GLN:HG2	1.90	0.53
2:B:275:ARG:HG2	2:B:368:CYS:SG	2.49	0.53
1:C:20:ARG:HH21	2:D:314:ARG:HD2	1.74	0.53
1:C:299:ARG:HH12	1:C:314:ARG:NH1	2.06	0.53
1:C:212:LYS:HA	1:C:215:SER:HB3	1.90	0.53
2:B:117:GLN:HA	2:B:120:GLU:CG	2.39	0.52
2:B:285:ASN:HB2	2:B:356:GLN:HB3	1.91	0.52
2:D:345:THR:HG22	2:D:351:SER:HA	1.90	0.52
1:A:211:PHE:O	1:A:215:SER:HB3	2.10	0.52
2:B:330:VAL:HG11	2:B:370:ILE:HB	1.92	0.52
2:B:26:PHE:HB3	2:B:185:LEU:HD13	1.91	0.52
2:B:147:TYR:HB2	2:B:167:VAL:HG21	1.91	0.52
2:B:189:GLN:HA	2:B:192:LYS:HE3	1.91	0.52
1:A:133:PHE:HE1	1:A:178:MET:HE2	1.75	0.51
2:D:44:MET:HG3	2:D:115:ILE:HD12	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:MET:HE3	1:C:111:MET:HG2	1.93	0.51
2:D:330:VAL:HG11	2:D:370:ILE:HB	1.92	0.51
1:C:44:MET:HG2	1:C:111:MET:HE2	1.92	0.50
1:A:46:ARG:NH2	2:B:53:GLU:OE2	2.42	0.50
2:D:234:GLN:O	2:D:238:VAL:HG13	2.10	0.50
1:C:219:ASN:OD1	1:C:220:GLU:N	2.45	0.50
2:B:44:MET:HG3	2:B:115:ILE:HD12	1.94	0.50
2:B:162:GLU:O	2:B:166:GLU:HG3	2.12	0.50
2:D:237:GLN:HG3	2:D:241:GLU:OE2	2.12	0.50
2:B:235:SER:O	2:B:238:VAL:HG22	2.12	0.49
2:D:190:TYR:HA	2:D:193:GLN:NE2	2.16	0.49
1:C:240:MET:HG3	2:D:190:TYR:CB	2.42	0.49
1:A:287:ARG:HD3	1:A:297:TRP:CZ2	2.48	0.48
1:C:190:TYR:HB2	2:D:240:LEU:HD12	1.93	0.48
2:D:328:CYS:SG	2:D:347:PRO:HD3	2.54	0.48
2:B:116:ILE:O	2:B:120:GLU:HG2	2.14	0.48
1:C:240:MET:SD	1:C:243:ASP:HB3	2.53	0.48
2:B:209:ASN:OD1	2:B:210:PHE:N	2.47	0.48
1:C:212:LYS:O	1:C:215:SER:HB3	2.13	0.48
1:A:265:ASP:HB2	2:B:147:TYR:OH	2.14	0.48
1:A:37:MET:HG3	1:A:118:PHE:HE2	1.79	0.47
1:C:140:HIS:HA	1:C:170:SER:HB3	1.96	0.47
1:C:151:SER:OG	2:D:337:ASP:OD2	2.23	0.47
1:C:9:ILE:HD12	1:C:10:GLU:HG3	1.96	0.47
1:C:117:GLN:O	1:C:121:ARG:HB2	2.15	0.47
2:D:238:VAL:HA	2:D:241:GLU:OE1	2.15	0.47
1:A:103:LEU:HD22	1:A:210:PHE:CG	2.50	0.47
2:B:309:LEU:HB2	2:B:325:LEU:HD11	1.95	0.47
1:A:288:ASN:N	1:A:288:ASN:OD1	2.47	0.47
2:D:330:VAL:HG13	2:D:367:ILE:HG23	1.97	0.47
1:A:193:LYS:NZ	2:B:79:ASP:HB3	2.30	0.46
2:B:37:THR:HG21	2:B:118:PHE:HE2	1.81	0.46
1:C:151:SER:O	1:C:155:GLU:HG3	2.15	0.46
1:C:225:PHE:O	1:C:229:ILE:HG12	2.15	0.46
1:C:227:ALA:O	1:C:231:THR:HG23	2.16	0.46
1:A:89:PHE:CD2	2:B:200:MET:HG2	2.51	0.46
2:B:149:ARG:HE	3:B:401:GOL:H31	1.81	0.46
2:D:284:LEU:HB2	2:D:302:PHE:CD1	2.51	0.45
2:D:128:THR:O	2:D:132:LEU:HG	2.17	0.45
1:C:23:LEU:O	1:C:27:GLU:HG3	2.16	0.45
1:A:201:LEU:HD12	2:B:226:LEU:HD22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PHE:O	1:A:229:ILE:HG12	2.16	0.45
2:B:116:ILE:HA	2:B:119:ARG:HG3	1.98	0.45
1:A:172:LYS:HG3	2:B:262:TYR:CE2	2.50	0.45
1:A:289:LYS:HA	1:A:295:SER:HA	1.99	0.45
1:C:215:SER:O	1:C:219:ASN:ND2	2.50	0.45
1:A:191:LYS:HG3	2:B:240:LEU:HD11	2.00	0.44
2:B:119:ARG:O	2:B:123:LEU:HB2	2.16	0.44
1:A:95:GLU:CD	1:A:221:GLN:HE22	2.25	0.44
1:C:193:LYS:HD3	2:D:82:VAL:HG11	1.99	0.44
1:A:23:LEU:O	1:A:27:GLU:HG3	2.18	0.44
1:C:165:GLU:O	1:C:165:GLU:HG2	2.16	0.44
1:C:336:GLU:O	1:C:337:ASP:HB2	2.17	0.44
1:C:338:ARG:HD2	1:C:356:GLN:NE2	2.32	0.44
2:D:265:ASP:OD2	2:D:340:TYR:OH	2.23	0.44
1:C:191:LYS:HG3	2:D:240:LEU:HD11	2.00	0.44
2:B:79:ASP:OD1	2:B:80:GLU:N	2.51	0.44
1:A:147:TYR:HB2	1:A:167:VAL:HG21	1.99	0.43
1:C:336:GLU:O	1:C:338:ARG:HG2	2.18	0.43
2:D:348:ASN:ND2	2:D:350:LYS:HG2	2.32	0.43
2:B:38:ASN:CG	2:B:119:ARG:HH12	2.26	0.43
2:B:120:GLU:HG2	2:B:120:GLU:H	1.66	0.43
1:C:20:ARG:HD2	2:D:314:ARG:HD2	1.99	0.43
2:D:111:MET:C	2:D:114:PRO:HD2	2.43	0.43
1:A:58:THR:HG22	1:A:93:ILE:HG23	2.01	0.43
1:C:211:PHE:CE1	2:D:214:GLY:HA3	2.53	0.43
1:C:156:ASN:HD21	1:C:159:VAL:H	1.67	0.43
2:B:68:TYR:O	2:B:71:GLN:HB3	2.18	0.43
1:A:25:VAL:HG13	2:B:74:ALA:HB1	1.99	0.43
1:A:151:SER:O	1:A:155:GLU:HG3	2.19	0.43
1:A:164:THR:HG23	2:B:264:PRO:HG2	1.99	0.43
2:B:217:MET:HE3	2:B:217:MET:HB2	1.85	0.43
2:B:237:GLN:O	2:B:240:LEU:HB3	2.19	0.43
2:B:107:LEU:O	2:B:111:MET:HB3	2.18	0.42
1:A:232:SER:CB	2:B:197:MET:HE1	2.47	0.42
1:C:225:PHE:CZ	2:D:200:MET:HB3	2.48	0.42
1:A:251:ILE:HD11	2:B:183:CYS:HB2	2.01	0.42
1:A:262:TYR:CE1	2:B:172:ARG:HA	2.54	0.42
2:B:72:ASN:O	2:B:73:PHE:HB2	2.19	0.42
1:C:124:LYS:HD3	1:C:124:LYS:HA	1.93	0.42
2:D:27:GLU:HG2	2:D:181:TYR:OH	2.18	0.42
1:A:9:ILE:H	1:A:9:ILE:HG13	1.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:MET:HG3	2:D:190:TYR:CG	2.54	0.42
2:D:44:MET:HB3	2:D:112:VAL:HG22	2.01	0.42
1:A:211:PHE:CE1	2:B:214:GLY:HA3	2.55	0.42
1:C:194:ILE:HD13	2:D:237:GLN:OE1	2.20	0.42
1:C:240:MET:CG	2:D:190:TYR:CG	3.03	0.42
1:C:152:LYS:NZ	2:D:334:ASP:OD1	2.35	0.42
1:A:125:GLU:HG3	1:A:129:LEU:HD13	2.02	0.42
1:C:240:MET:HG3	2:D:190:TYR:HB2	2.00	0.42
2:D:225:PHE:O	2:D:228:SER:OG	2.31	0.42
2:B:29:ASP:OD1	2:B:29:ASP:C	2.63	0.42
2:D:205:HIS:O	2:D:208:ILE:HG13	2.20	0.42
2:D:20:ARG:HD3	2:D:20:ARG:HA	1.81	0.41
1:A:287:ARG:HH11	1:A:354:ILE:HD12	1.85	0.41
2:B:111:MET:O	2:B:115:ILE:HG13	2.20	0.41
1:C:325:ILE:O	1:C:374:SER:HB2	2.20	0.41
1:A:251:ILE:O	1:A:255:GLU:HG3	2.20	0.41
2:B:325:LEU:HD22	2:B:370:ILE:HG23	2.02	0.41
1:A:244:ILE:HD13	1:A:244:ILE:HA	1.93	0.41
2:B:72:ASN:O	2:B:73:PHE:CB	2.68	0.41
2:B:284:LEU:HB2	2:B:302:PHE:CD1	2.55	0.41
1:C:62:SER:HB2	1:C:93:ILE:HG22	2.03	0.41
2:D:278:ILE:H	2:D:278:ILE:HG12	1.71	0.41
1:A:124:LYS:HD3	1:A:124:LYS:HA	1.93	0.41
1:A:280:LYS:HD3	1:A:366:TRP:CD2	2.56	0.41
1:A:227:ALA:O	1:A:231:THR:HG23	2.21	0.40
2:B:308:ASN:HB3	2:B:321:LEU:HD13	2.02	0.40
1:A:263:VAL:HA	1:A:264:PRO:HD2	1.88	0.40
1:C:285:ASN:HB2	1:C:356:GLN:HB3	2.03	0.40
2:D:309:LEU:O	2:D:322:ILE:HG22	2.21	0.40
2:D:300:LEU:HD22	2:D:313:PRO:HB3	2.03	0.40
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.96	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	352/375 (94%)	346 (98%)	6 (2%)	0	100	100
1	C	352/375 (94%)	343 (97%)	9 (3%)	0	100	100
2	B	368/375 (98%)	359 (98%)	8 (2%)	1 (0%)	36	65
2	D	369/375 (98%)	363 (98%)	6 (2%)	0	100	100
All	All	1441/1500 (96%)	1411 (98%)	29 (2%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	73	PHE

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	303/336 (90%)	293 (97%)	10 (3%)	33	67
1	C	300/336 (89%)	290 (97%)	10 (3%)	33	67
2	B	306/326 (94%)	294 (96%)	12 (4%)	28	63
2	D	298/326 (91%)	293 (98%)	5 (2%)	53	82
All	All	1207/1324 (91%)	1170 (97%)	37 (3%)	35	69

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	11	GLU
1	A	60	LEU
1	A	69	GLU
1	A	81	VAL
1	A	83	SER
1	A	117	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	146	ARG
1	A	212	LYS
1	A	249	GLN
2	B	29	ASP
2	B	120	GLU
2	B	121	LYS
2	B	146	LYS
2	B	159	VAL
2	B	162	GLU
2	B	234	GLN
2	B	245	GLU
2	B	249	VAL
2	B	252	GLN
2	B	266	SER
2	B	275	ARG
1	C	9	ILE
1	C	10	GLU
1	C	18	GLN
1	C	80	GLU
1	C	84	SER
1	C	102	VAL
1	C	117	GLN
1	C	159	VAL
1	C	165	GLU
1	C	317	VAL
2	D	146	LYS
2	D	208	ILE
2	D	241	GLU
2	D	252	GLN
2	D	353	ILE

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	189	GLN
1	A	308	ASN
2	B	59	GLN
2	B	138	ASN
2	B	193	GLN
2	B	323	GLN
1	C	18	GLN
1	C	51	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	305	GLN
1	C	308	ASN
2	D	87	HIS
2	D	97	ASN
2	D	193	GLN
2	D	285	ASN
2	D	343	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	401	-	5,5,5	0.54	0	5,5,5	0.61	0
3	GOL	D	401	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	B	401	-	5,5,5	0.37	0	5,5,5	0.30	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	GOL	A	401	-	-	0/4/4/4	-
3	GOL	D	401	-	-	2/4/4/4	-
3	GOL	B	401	-	-	2/4/4/4	-

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	B	401	GOL	O1-C1-C2-C3
3	D	401	GOL	O1-C1-C2-C3
3	B	401	GOL	O1-C1-C2-O2
3	D	401	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	GOL	1	0
3	B	401	GOL	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	358/375 (95%)	0.44	15 (4%)	40 32	37, 62, 102, 121	0
1	C	358/375 (95%)	0.40	14 (3%)	43 35	38, 63, 103, 121	0
2	B	370/375 (98%)	0.59	19 (5%)	33 26	38, 70, 105, 121	0
2	D	371/375 (98%)	0.40	13 (3%)	47 38	36, 65, 98, 121	0
All	All	1457/1500 (97%)	0.46	61 (4%)	40 32	36, 66, 102, 121	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	269	ALA	5.8
2	D	5	ASP	4.1
2	B	5	ASP	3.7
2	D	269	ALA	3.6
2	B	164	GLY	3.5
1	C	68	TYR	3.4
2	B	73	PHE	3.3
2	B	69	GLU	3.3
2	D	154	LYS	3.2
1	C	71	GLN	3.1
1	A	69	GLU	3.1
2	B	267	ASP	3.1
1	C	240	MET	3.0
1	A	11	GLU	3.0
1	A	70	LYS	3.0
2	D	151	PRO	3.0
2	B	80	GLU	2.9
1	A	289	LYS	2.9
1	C	337	ASP	2.9
2	B	53	GLU	2.8
2	B	159	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	156	ASN	2.7
2	D	150	LEU	2.7
2	B	291	GLY	2.6
1	A	358	GLU	2.6
1	A	268	PRO	2.6
2	B	307	GLY	2.5
2	B	74	ALA	2.5
1	A	319	GLY	2.5
1	A	180	HIS	2.4
2	D	291	GLY	2.4
2	D	290	THR	2.4
1	C	263	VAL	2.4
1	C	319	GLY	2.4
1	A	246	THR	2.4
2	B	196	MET	2.4
2	D	196	MET	2.3
1	A	337	ASP	2.3
1	A	68	TYR	2.3
2	D	36	TYR	2.3
2	B	328	CYS	2.3
1	A	190	TYR	2.3
2	D	153	LYS	2.3
1	C	90	SER	2.3
2	B	325	LEU	2.2
1	A	264	PRO	2.2
2	B	71	GLN	2.2
1	A	295	SER	2.2
1	A	248	GLN	2.1
2	B	249	VAL	2.1
1	C	295	SER	2.1
2	D	177	SER	2.1
2	D	184	ALA	2.1
1	C	154	ARG	2.1
2	B	184	ALA	2.1
2	D	155	GLU	2.1
2	B	176	LEU	2.1
1	C	4	MET	2.1
1	C	146	ARG	2.0
1	C	258	SER	2.0
1	C	335	CYS	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
3	GOL	B	401	6/6	0.67	0.17	77,85,88,90	0
3	GOL	A	401	6/6	0.73	0.16	72,98,99,103	0
3	GOL	D	401	6/6	0.76	0.16	64,76,83,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.