Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:22 PM GMT

PDB ID	:	1AGR
Title	:	COMPLEX OF ALF4-ACTIVATED GI-ALPHA-1 WITH RGS4
Authors	:	Tesmer, J.J.G.; Sprang, S.R.
Deposited on	:	1997-03-25
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

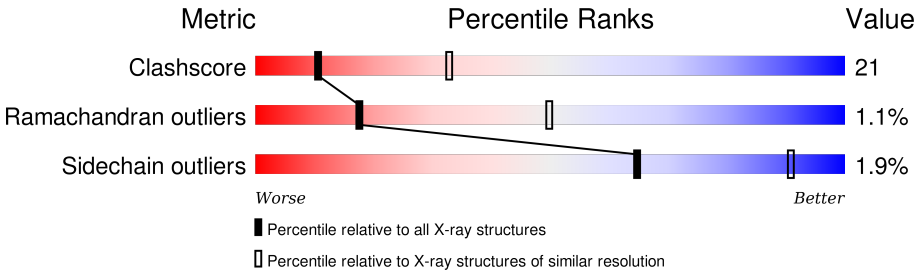
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	353	62% 36%
1	D	353	58% 38%
2	E	205	38% 23% 38%
2	H	205	26% 28% 43%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7732 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 GUANINE NUCLEOTIDE-BINDING PROTEIN G(I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2801	1772	477	535	17			
1	D	344	Total	C	N	O	S	0	0	0
			2759	1748	470	524	17			

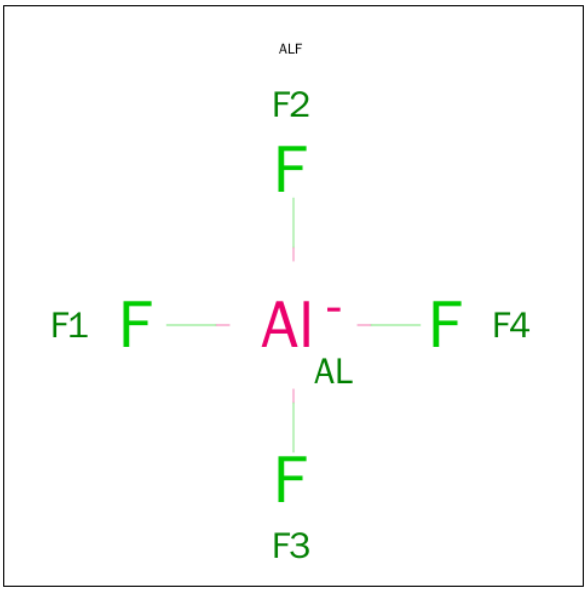
- Molecule 2 is a protein called RGS4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	128	Total	C	N	O	S	0	0	0
			1061	676	173	206	6			
2	H	116	Total	C	N	O	S	0	0	0
			959	611	157	185	6			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

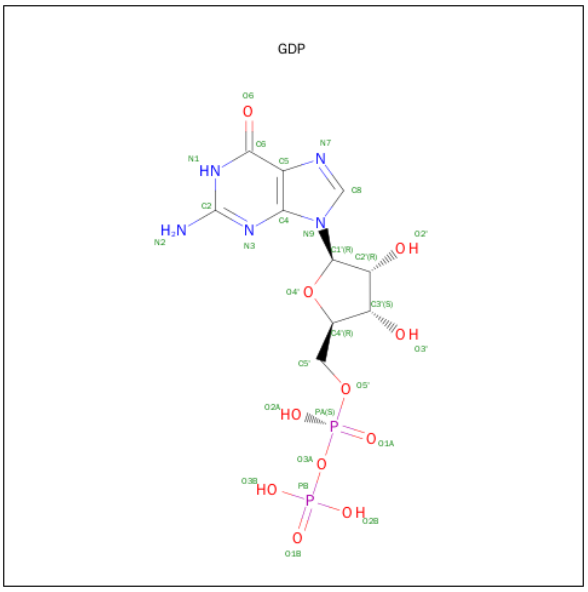
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Al	F		0	0
			5	1	4			
4	D	1	Total	Al	F		0	0
			5	1	4			

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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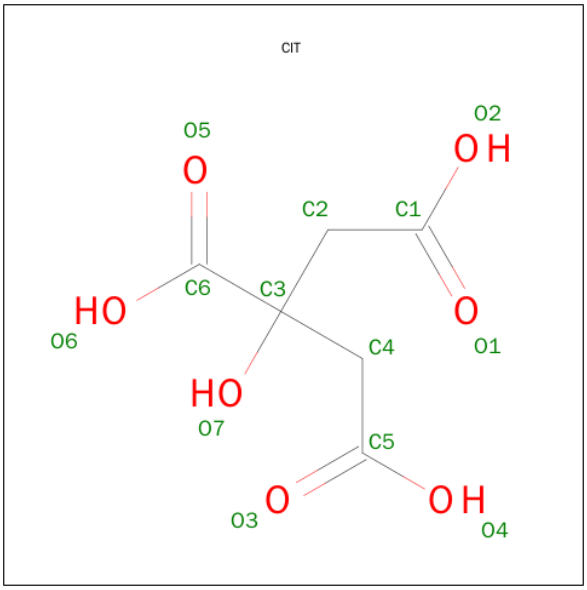
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 6 7	0	0
6	D	1	Total C O 13 6 7	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	26	Total O 26 26	0	0
7	D	26	Total O 26 26	0	0
7	E	3	Total O 3 3	0	0
7	H	3	Total O 3 3	0	0

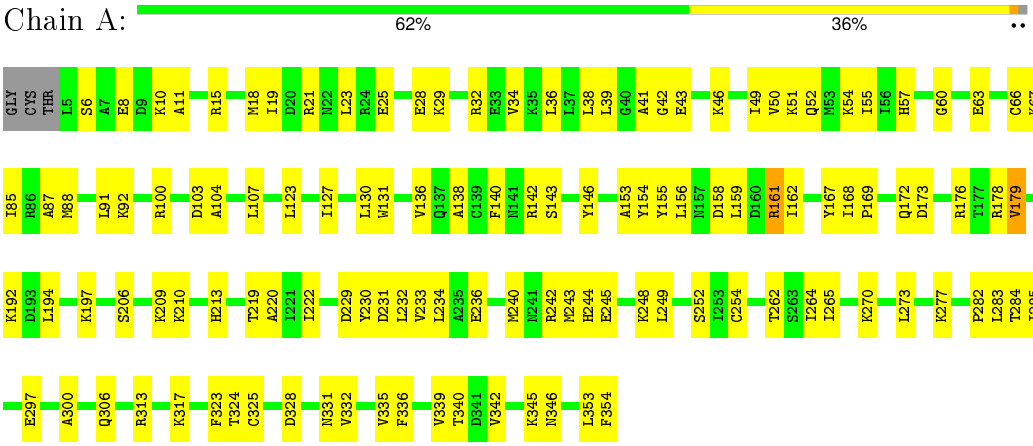
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

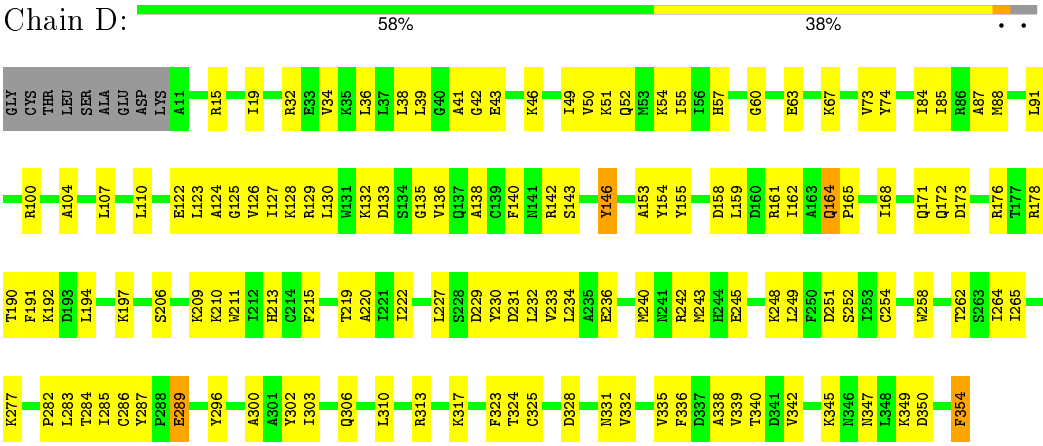
- Molecule 1: GUANINE NUCLEOTIDE-BINDING PROTEIN G(I)

Chain A:



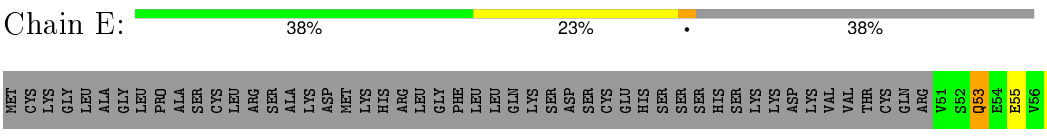
- Molecule 1: GUANINE NUCLEOTIDE-BINDING PROTEIN G(I)

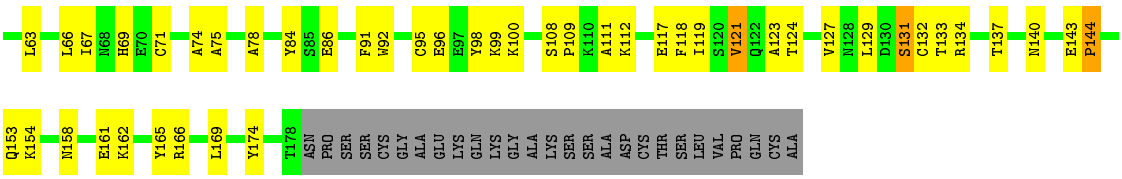
Chain D:



- Molecule 2: RGS4

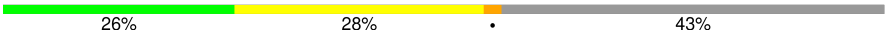
Chain E:

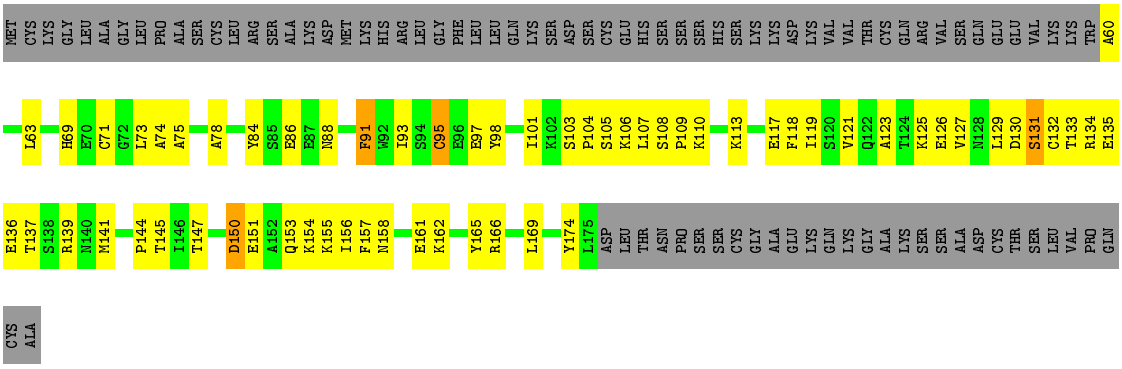




- Molecule 2: RGS4

Chain H:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	164.00Å 97.20Å 110.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.0 (5.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.216 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7732	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ALF, MG, CIT

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	0.55	0/2848	0.70	1/3832 (0.0%)
1	D	0.52	0/2806	0.67	0/3776
2	E	0.57	0/1081	0.66	0/1449
2	H	0.49	0/977	0.62	0/1308
All	All	0.54	0/7712	0.67	1/10365 (0.0%)

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	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	161	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	146	TYR	Sidechain

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	2801	0	2773	113	0
1	D	2759	0	2738	116	0
2	E	1061	0	1053	42	0
2	H	959	0	952	60	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	28	0	12	1	0
5	D	28	0	12	1	0
6	A	13	0	5	0	0
6	D	13	0	5	0	0
7	A	26	0	0	1	0
7	D	26	0	0	0	0
7	E	3	0	0	0	0
7	H	3	0	0	1	0
All	All	7732	0	7550	324	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 21.

All (324) 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:H:101:ILE:HD13	2:H:107:LEU:HA	1.39	1.02
1:A:36:LEU:HD11	1:A:222:ILE:HG13	1.47	0.95
1:D:36:LEU:HD11	1:D:222:ILE:HG13	1.50	0.91
1:D:128:LYS:HG2	1:D:159:LEU:HD23	1.52	0.88
2:E:59:TRP:HB3	2:E:66:LEU:HD12	1.56	0.86
2:E:154:LYS:NZ	2:E:154:LYS:HB3	1.96	0.81
1:A:55:ILE:HA	1:A:60:GLY:HA2	1.63	0.80
1:D:265:ILE:HD13	1:D:339:VAL:HG13	1.63	0.79
2:E:154:LYS:HZ2	2:E:154:LYS:HB3	1.47	0.79
2:E:118:PHE:O	2:E:127:VAL:HG22	1.85	0.77
2:E:98:TYR:CE1	2:E:111:ALA:HB2	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:THR:HA	1:A:287:TYR:O	1.84	0.77
1:D:284:THR:HA	1:D:287:TYR:O	1.85	0.76
1:D:55:ILE:HA	1:D:60:GLY:HA2	1.66	0.76
1:D:230:TYR:OH	1:D:277:LYS:HG2	1.87	0.75
1:A:230:TYR:OH	1:A:277:LYS:HG2	1.85	0.75
1:A:265:ILE:HD13	1:A:339:VAL:HG13	1.68	0.74
2:H:141:MET:O	2:H:144:PRO:HD3	1.86	0.74
2:H:118:PHE:O	2:H:127:VAL:HG22	1.88	0.73
2:H:73:LEU:HD21	2:H:93:ILE:HD11	1.69	0.72
2:H:73:LEU:HD11	2:H:93:ILE:HD11	1.71	0.72
1:A:100:ARG:HA	1:A:100:ARG:NE	2.05	0.72
2:H:101:ILE:HG21	2:H:107:LEU:N	2.05	0.71
2:H:106:LYS:C	2:H:109:PRO:HD2	2.11	0.71
2:H:101:ILE:HB	2:H:107:LEU:HD12	1.72	0.70
2:H:69:HIS:CE1	2:H:71:CYS:SG	2.85	0.70
1:D:191:PHE:CD2	1:D:340:THR:HG21	2.27	0.70
1:D:67:LYS:NZ	1:D:168:ILE:HD13	2.07	0.69
2:H:97:GLU:HB3	2:H:110:LYS:HE3	1.74	0.69
2:E:117:GLU:O	2:E:123:ALA:HB1	1.93	0.69
1:A:287:TYR:CE2	1:A:306:GLN:HG3	2.29	0.68
1:D:270:LYS:HD2	1:D:273:LEU:HD12	1.75	0.68
2:E:59:TRP:HB3	2:E:66:LEU:CD1	2.23	0.68
1:A:143:SER:HA	1:A:146:TYR:CE1	2.29	0.67
1:D:191:PHE:HD2	1:D:340:THR:HG21	1.60	0.66
1:A:85:ILE:HG12	1:A:88:MET:CE	2.25	0.66
1:A:57:HIS:HE1	1:A:336:PHE:CD2	2.14	0.66
1:A:191:PHE:CD2	1:A:340:THR:HG21	2.30	0.66
1:A:18:MET:HA	1:A:21:ARG:NH1	2.10	0.66
2:H:158:ASN:OD1	2:H:162:LYS:HE2	1.96	0.66
1:A:88:MET:HE1	1:A:136:VAL:HG22	1.78	0.65
1:A:270:LYS:HD2	1:A:273:LEU:HD12	1.78	0.65
1:D:63:GLU:O	1:D:67:LYS:HG3	1.97	0.65
1:A:63:GLU:O	1:A:67:LYS:HG3	1.96	0.64
2:H:161:GLU:HG2	2:H:166:ARG:HH21	1.62	0.64
1:A:162:ILE:HA	1:A:167:TYR:CD2	2.32	0.64
2:H:151:GLU:OE2	2:H:155:LYS:HE3	1.98	0.64
1:D:57:HIS:HE1	1:D:336:PHE:CD2	2.17	0.63
1:A:336:PHE:O	1:A:340:THR:HG23	1.97	0.63
1:D:143:SER:HA	1:D:146:TYR:CE1	2.33	0.63
2:E:161:GLU:HG2	2:E:166:ARG:HH21	1.64	0.62
1:A:264:ILE:HD12	1:A:317:LYS:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:69:HIS:CE1	2:E:71:CYS:SG	2.93	0.62
1:D:190:THR:HG23	1:D:194:LEU:O	2.00	0.62
2:E:158:ASN:OD1	2:E:162:LYS:HE2	2.00	0.62
1:A:331:ASN:O	1:A:335:VAL:HG23	1.99	0.61
2:H:117:GLU:O	2:H:123:ALA:HB1	1.99	0.61
2:H:91:PHE:HE1	2:H:153:GLN:HA	1.64	0.61
1:D:349:LYS:HE2	1:D:354:PHE:CD2	2.35	0.61
1:A:234:LEU:HD21	1:A:245:GLU:HG2	1.82	0.61
1:D:178:ARG:HD2	1:D:179:VAL:H	1.66	0.60
1:D:349:LYS:HE2	1:D:354:PHE:CE2	2.37	0.59
1:D:188:HIS:NE2	1:D:197:LYS:HG2	2.16	0.59
1:D:67:LYS:HG2	1:D:168:ILE:HG23	1.85	0.59
1:D:178:ARG:HD2	1:D:179:VAL:N	2.18	0.59
1:A:229:ASP:HB3	1:A:242:ARG:HB2	1.83	0.59
2:H:101:ILE:CD1	2:H:107:LEU:HA	2.25	0.59
1:D:125:GLY:O	1:D:129:ARG:HG3	2.03	0.59
1:D:234:LEU:HD21	1:D:245:GLU:HG2	1.85	0.59
1:A:188:HIS:NE2	1:A:197:LYS:HG2	2.17	0.59
1:A:191:PHE:O	1:A:194:LEU:HB2	2.03	0.59
1:D:264:ILE:HD12	1:D:317:LYS:HE3	1.85	0.59
1:D:331:ASN:O	1:D:335:VAL:HG23	2.03	0.58
1:D:347:ASN:O	1:D:350:ASP:HB2	2.03	0.58
1:A:28:GLU:OE1	1:A:353:LEU:HD13	2.03	0.58
1:D:122:GLU:O	1:D:126:VAL:HG23	2.03	0.58
1:D:210:LYS:HD3	2:H:84:TYR:O	2.04	0.57
1:A:172:GLN:HE21	1:A:172:GLN:HA	1.69	0.57
2:E:95:CYS:O	2:E:99:LYS:HG3	2.04	0.57
1:A:85:ILE:HG12	1:A:88:MET:HE3	1.86	0.57
1:D:229:ASP:HB3	1:D:242:ARG:HB2	1.85	0.57
2:H:98:TYR:HE2	2:H:145:THR:O	1.87	0.57
1:A:178:ARG:HD2	1:A:179:VAL:N	2.20	0.57
1:A:161:ARG:NH2	1:A:173:ASP:OD2	2.38	0.56
1:D:104:ALA:O	1:D:107:LEU:HB3	2.05	0.56
2:H:165:TYR:CZ	2:H:169:LEU:HD11	2.40	0.56
2:H:71:CYS:O	2:H:74:ALA:HB3	2.05	0.56
2:H:101:ILE:HB	2:H:107:LEU:CD1	2.36	0.56
2:H:101:ILE:HG21	2:H:107:LEU:CA	2.36	0.56
2:E:98:TYR:CZ	2:E:111:ALA:HB2	2.41	0.56
2:H:151:GLU:O	2:H:154:LYS:HB3	2.05	0.56
1:D:110:LEU:HD13	1:D:123:LEU:HA	1.88	0.55
1:D:172:GLN:O	1:D:176:ARG:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:LYS:O	1:D:349:LYS:HG3	2.06	0.55
1:A:73:VAL:HG13	1:A:155:TYR:CE1	2.41	0.55
2:E:53:GLN:O	2:E:57:LYS:HG3	2.07	0.55
1:D:172:GLN:HA	1:D:172:GLN:NE2	2.22	0.55
1:A:335:VAL:O	1:A:339:VAL:HG23	2.07	0.55
1:D:213:HIS:CG	2:H:84:TYR:CE2	2.95	0.55
1:A:178:ARG:HD2	1:A:179:VAL:H	1.72	0.55
1:D:38:LEU:O	1:D:39:LEU:HD23	2.07	0.54
2:H:97:GLU:CB	2:H:110:LYS:HE3	2.35	0.54
1:D:172:GLN:HA	1:D:172:GLN:HE21	1.70	0.54
1:D:130:LEU:O	1:D:136:VAL:HG21	2.07	0.54
1:A:38:LEU:O	1:A:39:LEU:HD23	2.08	0.54
1:A:191:PHE:CE2	1:A:340:THR:HG21	2.43	0.54
1:D:287:TYR:CE2	1:D:306:GLN:HG3	2.43	0.54
1:D:188:HIS:CD2	1:D:197:LYS:HG2	2.42	0.54
2:H:153:GLN:O	2:H:153:GLN:HG2	2.07	0.54
1:A:172:GLN:O	1:A:176:ARG:HG2	2.07	0.54
1:A:172:GLN:NE2	1:A:172:GLN:HA	2.23	0.54
1:D:176:ARG:NH1	5:D:355:GDP:HN22	2.06	0.54
1:A:123:LEU:O	1:A:127:ILE:HG13	2.08	0.54
1:A:345:LYS:HG2	1:A:354:PHE:HE1	1.72	0.53
2:H:95:CYS:SG	2:H:153:GLN:HB2	2.49	0.53
2:E:108:SER:O	2:E:112:LYS:HG3	2.07	0.53
1:A:19:ILE:O	1:A:23:LEU:HD12	2.08	0.53
1:A:138:ALA:O	1:A:142:ARG:HG3	2.08	0.53
1:A:249:LEU:O	1:A:252:SER:HB3	2.08	0.53
1:A:178:ARG:O	1:A:179:VAL:HG23	2.09	0.53
1:D:100:ARG:HH11	1:D:100:ARG:HG2	1.74	0.53
1:A:230:TYR:O	1:A:286:CYS:HB2	2.09	0.52
2:H:73:LEU:HD21	2:H:93:ILE:CD1	2.36	0.52
1:D:158:ASP:HB3	1:D:161:ARG:NH1	2.24	0.52
1:D:39:LEU:O	1:D:46:LYS:HD3	2.09	0.52
1:D:231:ASP:O	1:D:232:LEU:HD23	2.08	0.52
1:D:85:ILE:HD11	1:D:130:LEU:HD13	1.91	0.52
1:D:289:GLU:HA	1:D:289:GLU:OE1	2.09	0.52
2:H:136:GLU:HA	2:H:139:ARG:NH1	2.25	0.52
1:D:230:TYR:CE1	1:D:277:LYS:HD2	2.43	0.52
1:A:57:HIS:HE1	1:A:336:PHE:HD2	1.57	0.52
1:A:176:ARG:NH1	5:A:355:GDP:HN22	2.08	0.52
2:E:165:TYR:CZ	2:E:169:LEU:HD11	2.45	0.52
2:H:91:PHE:CE1	2:H:153:GLN:HA	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:PHE:HD2	1:A:340:THR:HG21	1.73	0.51
2:H:60:ALA:HB2	2:H:174:TYR:OH	2.09	0.51
1:A:265:ILE:HD13	1:A:339:VAL:CG1	2.40	0.51
1:D:270:LYS:CD	1:D:273:LEU:HD12	2.40	0.51
1:A:213:HIS:CG	2:E:84:TYR:CE2	2.99	0.51
1:A:270:LYS:CD	1:A:273:LEU:HD12	2.41	0.51
1:A:210:LYS:HD3	2:E:84:TYR:O	2.10	0.51
1:D:178:ARG:O	1:D:179:VAL:HG23	2.10	0.51
1:D:73:VAL:HG13	1:D:155:TYR:CE1	2.46	0.51
1:D:230:TYR:O	1:D:286:CYS:HB2	2.11	0.51
1:A:230:TYR:CE1	1:A:277:LYS:HD2	2.46	0.51
1:A:100:ARG:HD3	1:A:130:LEU:HD23	1.93	0.50
2:H:147:THR:HA	2:H:150:ASP:OD1	2.12	0.50
2:H:147:THR:O	2:H:150:ASP:HB2	2.10	0.50
1:A:91:LEU:O	1:A:92:LYS:HB3	2.12	0.50
1:D:15:ARG:O	1:D:19:ILE:HG13	2.12	0.50
1:A:25:GLU:O	1:A:29:LYS:HG3	2.12	0.50
2:E:91:PHE:HE2	2:E:153:GLN:HA	1.77	0.50
1:A:85:ILE:O	1:A:88:MET:HB2	2.11	0.49
1:A:52:GLN:HG3	1:A:332:VAL:HG21	1.94	0.49
1:D:38:LEU:HD12	1:D:50:VAL:HG23	1.95	0.49
1:D:100:ARG:HG2	1:D:100:ARG:NH1	2.27	0.49
1:D:236:GLU:HA	2:H:131:SER:H	1.76	0.49
1:A:289:GLU:OE1	1:A:289:GLU:HA	2.13	0.49
2:E:55:GLU:CG	2:E:69:HIS:HD2	2.26	0.49
1:A:188:HIS:CD2	1:A:197:LYS:HG2	2.48	0.49
1:D:254:CYS:HA	1:D:264:ILE:HD13	1.95	0.49
2:E:96:GLU:O	2:E:100:LYS:HG2	2.13	0.48
1:A:38:LEU:HD12	1:A:50:VAL:HG23	1.95	0.48
2:E:92:TRP:O	2:E:96:GLU:HG2	2.12	0.48
2:E:59:TRP:CB	2:E:66:LEU:HD12	2.37	0.48
2:H:69:HIS:HE1	2:H:71:CYS:SG	2.35	0.48
1:A:39:LEU:O	1:A:46:LYS:HD3	2.14	0.48
1:D:91:LEU:O	1:D:92:LYS:HB2	2.13	0.48
2:H:98:TYR:CE2	2:H:145:THR:O	2.66	0.48
2:E:119:ILE:HG21	2:E:137:THR:HG21	1.96	0.48
1:D:128:LYS:O	1:D:132:LYS:HG2	2.14	0.48
1:D:127:ILE:HG22	1:D:159:LEU:HD22	1.94	0.48
1:D:138:ALA:O	1:D:142:ARG:HG3	2.13	0.48
1:D:282:PRO:HG2	1:D:285:ILE:HG13	1.95	0.48
1:D:338:ALA:O	1:D:342:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:LEU:HD21	2:H:156:ILE:HD12	1.96	0.47
2:E:59:TRP:CZ2	2:E:71:CYS:HB2	2.49	0.47
1:A:236:GLU:HA	2:E:131:SER:H	1.79	0.47
1:D:133:ASP:OD2	1:D:135:GLY:N	2.47	0.47
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.78	0.47
2:H:161:GLU:HG2	2:H:166:ARG:NH2	2.29	0.47
1:A:233:VAL:HA	1:A:240:MET:O	2.14	0.47
2:E:71:CYS:O	2:E:74:ALA:HB3	2.14	0.47
2:E:95:CYS:SG	2:E:153:GLN:HG3	2.55	0.47
1:D:233:VAL:HA	1:D:240:MET:O	2.14	0.47
2:H:104:PRO:HG2	2:H:105:SER:H	1.80	0.47
2:H:108:SER:N	2:H:109:PRO:CD	2.78	0.47
2:H:98:TYR:HD1	2:H:110:LYS:HB3	1.79	0.47
1:A:231:ASP:O	1:A:232:LEU:HD23	2.14	0.47
1:D:249:LEU:O	1:D:252:SER:HB3	2.15	0.47
1:A:206:SER:O	1:A:209:LYS:HE3	2.13	0.47
2:H:104:PRO:C	2:H:106:LYS:H	2.19	0.47
2:E:98:TYR:OH	2:E:111:ALA:HB2	2.15	0.47
2:H:95:CYS:HB3	2:H:153:GLN:OE1	2.15	0.47
1:D:110:LEU:HD21	1:D:122:GLU:OE1	2.16	0.46
1:D:154:TYR:CE1	1:D:176:ARG:HG3	2.50	0.46
1:A:51:LYS:O	1:A:54:LYS:HB3	2.15	0.46
1:D:49:ILE:O	1:D:52:GLN:HB2	2.15	0.46
1:D:88:MET:HE1	1:D:136:VAL:HG22	1.96	0.46
1:A:282:PRO:HG2	1:A:285:ILE:HG13	1.97	0.46
1:D:57:HIS:HE1	1:D:336:PHE:HD2	1.62	0.46
1:A:219:THR:O	1:A:262:THR:HG23	2.15	0.46
1:A:191:PHE:CZ	1:A:192:LYS:HE3	2.51	0.46
1:A:28:GLU:O	1:A:32:ARG:HG2	2.16	0.46
1:D:43:GLU:CD	1:D:242:ARG:HH12	2.19	0.46
1:D:88:MET:HE1	1:D:95:PHE:CE1	2.51	0.46
1:A:283:LEU:O	1:A:283:LEU:HG	2.16	0.46
1:D:36:LEU:HA	1:D:220:ALA:O	2.16	0.46
1:A:328:ASP:O	1:A:332:VAL:HG23	2.16	0.46
1:D:219:THR:O	1:D:262:THR:HG23	2.16	0.46
1:D:110:LEU:HB3	1:D:123:LEU:HD13	1.98	0.45
1:A:297:GLU:HG3	1:D:296:TYR:HE2	1.80	0.45
1:D:74:TYR:CE1	1:D:162:ILE:O	2.69	0.45
2:H:101:ILE:HG23	2:H:106:LYS:HB3	1.97	0.45
1:A:242:ARG:HB3	7:A:372:HOH:O	2.16	0.45
2:E:95:CYS:CB	2:E:153:GLN:HG3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:SER:HA	1:A:146:TYR:CD1	2.52	0.45
1:A:127:ILE:HB	1:A:159:LEU:HD21	1.97	0.45
1:D:227:LEU:HD23	1:D:303:ILE:HG21	1.98	0.45
2:H:63:LEU:HD23	2:H:157:PHE:CE1	2.52	0.45
1:D:34:VAL:HG13	1:D:219:THR:HG21	1.99	0.45
1:D:39:LEU:C	1:D:46:LYS:HD3	2.37	0.45
1:A:345:LYS:HG2	1:A:354:PHE:CE1	2.50	0.45
1:A:34:VAL:HA	1:A:219:THR:OG1	2.17	0.45
1:D:215:PHE:O	1:D:258:TRP:CE3	2.70	0.45
2:H:137:THR:O	2:H:141:MET:HG2	2.17	0.44
1:D:74:TYR:HE1	1:D:162:ILE:O	2.00	0.44
1:D:51:LYS:O	1:D:54:LYS:HB3	2.17	0.44
1:D:302:TYR:O	1:D:306:GLN:HG2	2.17	0.44
1:A:88:MET:CE	1:A:136:VAL:HG22	2.46	0.44
2:E:91:PHE:HA	2:E:118:PHE:CE2	2.52	0.44
1:D:191:PHE:O	1:D:194:LEU:HB2	2.17	0.44
1:A:154:TYR:CE1	1:A:176:ARG:HG3	2.53	0.44
2:E:161:GLU:HG2	2:E:166:ARG:NH2	2.32	0.44
1:D:46:LYS:O	1:D:50:VAL:HG23	2.18	0.44
2:E:108:SER:N	2:E:109:PRO:HD2	2.33	0.44
1:D:211:TRP:CZ3	1:D:249:LEU:HD11	2.53	0.44
2:H:98:TYR:OH	2:H:144:PRO:HB3	2.17	0.44
1:A:161:ARG:HH22	1:A:173:ASP:CG	2.21	0.44
1:D:85:ILE:CD1	1:D:130:LEU:HD13	2.46	0.44
1:D:84:ILE:O	1:D:87:ALA:HB3	2.17	0.44
1:D:67:LYS:HG2	1:D:168:ILE:CG2	2.47	0.44
1:A:39:LEU:C	1:A:46:LYS:HD3	2.38	0.44
1:A:342:VAL:HG12	1:A:346:ASN:ND2	2.32	0.44
2:H:103:SER:OG	2:H:104:PRO:HD2	2.18	0.44
1:D:206:SER:O	1:D:209:LYS:HE3	2.17	0.44
2:E:55:GLU:CG	2:E:69:HIS:CD2	3.01	0.44
2:H:130:ASP:OD2	2:H:132:CYS:SG	2.75	0.44
1:D:230:TYR:HA	1:D:243:MET:HB2	2.00	0.43
1:A:230:TYR:HA	1:A:243:MET:HB2	1.99	0.43
1:A:100:ARG:O	1:A:103:ASP:N	2.51	0.43
1:D:240:MET:HE3	1:D:248:LYS:HZ2	1.83	0.43
1:A:34:VAL:HG13	1:A:219:THR:HB	2.00	0.43
1:A:8:GLU:O	1:A:11:ALA:HB3	2.18	0.43
2:H:129:LEU:HD22	2:H:133:THR:HG21	2.00	0.43
1:D:328:ASP:O	1:D:332:VAL:HG23	2.18	0.43
2:E:129:LEU:HD22	2:E:133:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:119:ILE:HG21	2:H:137:THR:HG21	1.99	0.43
1:A:100:ARG:HG2	1:A:100:ARG:NH1	2.33	0.43
1:A:46:LYS:O	1:A:50:VAL:HG23	2.19	0.43
1:D:140:PHE:CZ	1:D:153:ALA:HB2	2.53	0.43
1:A:140:PHE:CZ	1:A:153:ALA:HB2	2.54	0.43
1:A:240:MET:HE3	1:A:248:LYS:HZ2	1.83	0.43
2:E:75:ALA:O	2:E:78:ALA:HB3	2.19	0.43
1:D:143:SER:HA	1:D:146:TYR:CD1	2.54	0.43
2:E:132:CYS:SG	2:E:133:THR:N	2.92	0.43
1:A:66:CYS:HB3	1:A:169:PRO:O	2.18	0.43
2:H:88:ASN:ND2	7:H:208:HOH:O	2.47	0.43
1:D:191:PHE:CZ	1:D:192:LYS:HG3	2.53	0.43
1:D:191:PHE:CZ	1:D:192:LYS:HE3	2.53	0.43
1:D:161:ARG:NH2	1:D:173:ASP:OD2	2.52	0.43
1:A:34:VAL:HG13	1:A:219:THR:HG21	2.00	0.43
1:A:313:ARG:O	1:A:317:LYS:HB3	2.18	0.43
1:A:162:ILE:HA	1:A:167:TYR:CE2	2.54	0.42
2:E:60:ALA:HB2	2:E:174:TYR:CZ	2.54	0.42
1:D:34:VAL:HG13	1:D:219:THR:HB	2.02	0.42
2:H:129:LEU:HD21	2:H:156:ILE:CD1	2.50	0.42
1:A:324:THR:HA	1:A:331:ASN:OD1	2.20	0.42
2:H:123:ALA:HB3	2:H:126:GLU:HB2	2.02	0.42
2:E:53:GLN:HE21	2:E:53:GLN:HA	1.84	0.42
1:A:6:SER:O	1:A:10:LYS:HB2	2.20	0.42
1:D:161:ARG:NH2	1:D:173:ASP:OD1	2.51	0.42
1:D:42:GLY:O	1:D:43:GLU:HB2	2.19	0.42
1:A:49:ILE:O	1:A:52:GLN:HB2	2.18	0.42
1:D:52:GLN:HG3	1:D:332:VAL:HG21	2.02	0.42
1:A:100:ARG:NE	1:A:100:ARG:CA	2.80	0.42
1:D:324:THR:HA	1:D:331:ASN:OD1	2.20	0.42
1:A:73:VAL:HG13	1:A:155:TYR:CD1	2.54	0.42
2:E:121:VAL:HG23	2:E:134:ARG:HD2	2.02	0.42
1:A:36:LEU:HA	1:A:220:ALA:O	2.20	0.42
1:D:93:ILE:HD11	1:D:142:ARG:HD3	2.00	0.42
1:D:265:ILE:CD1	1:D:339:VAL:HG13	2.41	0.42
1:A:190:THR:HG23	1:A:194:LEU:O	2.20	0.42
1:D:231:ASP:C	1:D:232:LEU:HD23	2.41	0.41
1:A:300:ALA:HB1	1:A:323:PHE:HE2	1.85	0.41
1:D:124:ALA:O	1:D:128:LYS:HG3	2.20	0.41
1:A:254:CYS:HA	1:A:264:ILE:HD13	2.00	0.41
2:H:75:ALA:O	2:H:78:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:TYR:CZ	1:A:306:GLN:HG3	2.55	0.41
1:D:283:LEU:O	1:D:283:LEU:HG	2.19	0.41
2:H:121:VAL:HG23	2:H:134:ARG:HD2	2.01	0.41
1:A:244:HIS:CD2	1:A:286:CYS:HG	2.38	0.41
1:A:104:ALA:O	1:A:107:LEU:HB3	2.21	0.41
1:A:42:GLY:O	1:A:43:GLU:HB2	2.21	0.41
2:H:131:SER:O	2:H:135:GLU:HG3	2.20	0.41
2:H:101:ILE:HG12	2:H:106:LYS:HG2	2.02	0.41
1:D:313:ARG:O	1:D:317:LYS:HB3	2.20	0.41
1:A:131:TRP:CE3	1:A:156:LEU:HD13	2.56	0.41
2:E:143:GLU:N	2:E:144:PRO:HD3	2.36	0.41
1:D:164:GLN:HA	1:D:165:PRO:HD3	1.89	0.41
2:H:118:PHE:HE1	2:H:125:LYS:HE2	1.86	0.41
1:A:67:LYS:NZ	1:A:168:ILE:HD13	2.36	0.41
1:D:300:ALA:HB1	1:D:323:PHE:HE2	1.86	0.41
1:D:32:ARG:HA	1:D:194:LEU:CD2	2.51	0.40
1:A:85:ILE:HA	1:A:88:MET:HE3	2.02	0.40
2:H:91:PHE:HE2	2:H:119:ILE:HD11	1.86	0.40
1:A:43:GLU:CD	1:A:242:ARG:HH12	2.24	0.40
1:A:34:VAL:HG13	1:A:219:THR:CG2	2.51	0.40
1:D:34:VAL:HG13	1:D:219:THR:CG2	2.51	0.40
1:D:251:ASP:HB2	1:D:310:LEU:HD22	2.02	0.40
2:E:63:LEU:O	2:E:67:ILE:HG12	2.21	0.40
1:D:230:TYR:HE1	1:D:277:LYS:HD2	1.87	0.40
2:E:137:THR:O	2:E:140:ASN:HB2	2.22	0.40
1:A:84:ILE:O	1:A:87:ALA:HB3	2.20	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	348/353 (99%)	318 (91%)	28 (8%)	2 (1%)	30 65
1	D	342/353 (97%)	314 (92%)	25 (7%)	3 (1%)	21 55
2	E	126/205 (62%)	113 (90%)	10 (8%)	3 (2%)	7 25
2	H	114/205 (56%)	93 (82%)	19 (17%)	2 (2%)	11 34
All	All	930/1116 (83%)	838 (90%)	82 (9%)	10 (1%)	17 50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	41	ALA
1	A	41	ALA
1	A	179	VAL
1	D	179	VAL
2	E	144	PRO
2	H	131	SER
2	E	124	THR
1	D	92	LYS
2	H	113	LYS
2	E	131	SER

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	300/303 (99%)	296 (99%)	4 (1%)	76 94
1	D	296/303 (98%)	291 (98%)	5 (2%)	68 92
2	E	120/185 (65%)	117 (98%)	3 (2%)	55 86
2	H	108/185 (58%)	104 (96%)	4 (4%)	41 76
All	All	824/976 (84%)	808 (98%)	16 (2%)	65 91

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG

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Mol	Chain	Res	Type
1	A	158	ASP
1	A	289	GLU
1	A	325	CYS
1	D	164	GLN
1	D	171	GLN
1	D	289	GLU
1	D	325	CYS
1	D	354	PHE
2	E	53	GLN
2	E	86	GLU
2	E	121	VAL
2	H	86	GLU
2	H	91	PHE
2	H	95	CYS
2	H	150	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	57	HIS
1	A	172	GLN
1	D	57	HIS
1	D	164	GLN
1	D	172	GLN
2	E	53	GLN
2	E	69	HIS
2	E	88	ASN
2	H	69	HIS
2	H	88	ASN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
5	GDP	A	355	3,4	23,30,30	1.91	6 (26%)	30,47,47	2.82	12 (40%)
4	ALF	A	357	1,3,5,7	0,4,4	0.00	-	0,6,6	0.00	-
6	CIT	A	358	-	3,12,12	1.06	0	3,17,17	2.08	1 (33%)
5	GDP	D	355	3,4	23,30,30	1.66	3 (13%)	30,47,47	2.81	9 (30%)
4	ALF	D	357	1,3,5,7	0,4,4	0.00	-	0,6,6	0.00	-
6	CIT	D	358	-	3,12,12	0.79	0	3,17,17	2.35	1 (33%)

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
5	GDP	A	355	3,4	-	0/12/32/32	0/3/3/3
4	ALF	A	357	1,3,5,7	-	0/0/0/0	0/0/0/0
6	CIT	A	358	-	-	0/6/16/16	0/0/0/0
5	GDP	D	355	3,4	-	0/12/32/32	0/3/3/3
4	ALF	D	357	1,3,5,7	-	0/0/0/0	0/0/0/0
6	CIT	D	358	-	-	0/6/16/16	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	355	GDP	C8-N7	-2.94	1.29	1.34
5	D	355	GDP	C8-N7	-2.82	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	355	GDP	O5'-C5'	-2.14	1.36	1.44
5	A	355	GDP	C3'-C4'	-2.06	1.47	1.53
5	D	355	GDP	C2-N1	2.26	1.39	1.35
5	A	355	GDP	C2-N1	2.76	1.40	1.35
5	A	355	GDP	O4'-C1'	3.63	1.45	1.41
5	A	355	GDP	C6-N1	4.62	1.41	1.33
5	D	355	GDP	C6-N1	5.20	1.42	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	355	GDP	C5-C6-N1	-9.62	110.44	123.59
5	A	355	GDP	C5-C6-N1	-9.26	110.92	123.59
5	A	355	GDP	PA-O3A-PB	-4.41	117.90	132.67
5	D	355	GDP	PA-O3A-PB	-3.91	119.57	132.67
5	D	355	GDP	N3-C2-N1	-3.67	121.86	127.44
5	A	355	GDP	N3-C2-N1	-2.65	123.40	127.44
5	A	355	GDP	O3'-C3'-C2'	-2.37	104.11	111.83
5	A	355	GDP	C1'-N9-C4	-2.13	123.73	126.94
5	D	355	GDP	O3'-C3'-C2'	-2.04	105.19	111.83
5	D	355	GDP	O2B-PB-O1B	2.03	117.12	110.58
5	A	355	GDP	C4-C5-N7	2.04	111.35	109.48
5	A	355	GDP	N2-C2-N1	2.05	120.60	117.20
5	D	355	GDP	O2A-PA-O3A	2.36	115.79	105.09
5	D	355	GDP	C4'-O4'-C1'	2.43	112.39	109.72
5	A	355	GDP	O2B-PB-O1B	2.66	119.16	110.58
6	A	358	CIT	C3-C2-C1	3.07	119.86	114.96
5	A	355	GDP	O2A-PA-O3A	3.29	120.03	105.09
6	D	358	CIT	C3-C2-C1	3.68	120.84	114.96
5	A	355	GDP	C4'-O4'-C1'	3.71	113.80	109.72
5	A	355	GDP	C2'-C1'-N9	4.28	120.83	114.29
5	D	355	GDP	C2'-C1'-N9	4.47	121.13	114.29
5	A	355	GDP	C6-N1-C2	6.84	125.43	115.94
5	D	355	GDP	C6-N1-C2	7.37	126.16	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	355	GDP	1	0
5	D	355	GDP	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.