Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:22 PM GMT

PDB ID	:	1TBG
Title	:	BETA-GAMMA DIMER OF THE HETEROTRIMERIC G-PROTEIN TRANSDUCIN
Authors	:	Sondek, J.S.; Bohm, A.; Lambright, D.G.; Hamm, H.E.; Sigler, P.B.
Deposited on	:	1996-06-15
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

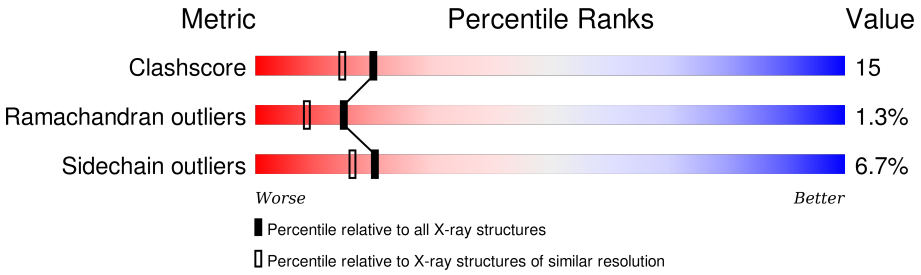
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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 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	340	68% 30% ·
1	B	340	64% 33% ·
1	C	340	66% 31% ·
1	D	340	64% 35% ·
2	E	68	62% 34% ·
2	F	68	65% 25% 6% ·
2	G	68	62% 29% · ·

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Mol	Chain	Length	Quality of chain
2	H	68	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13273 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 TRANSDUCIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2615	1612	469	512	22			
1	B	340	Total	C	N	O	S	0	0	0
			2615	1612	469	512	22			
1	C	340	Total	C	N	O	S	0	0	0
			2615	1612	469	512	22			
1	D	340	Total	C	N	O	S	0	0	0
			2615	1612	469	512	22			

- Molecule 2 is a protein called TRANSDUCIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	68	Total	C	N	O	S	0	0	0
			524	325	87	108	4			
2	F	65	Total	C	N	O	S	0	0	0
			518	324	85	105	4			
2	G	65	Total	C	N	O	S	0	0	0
			527	330	86	107	4			
2	H	65	Total	C	N	O	S	0	0	0
			512	319	85	104	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	108	Total	O	0	0
			108	108		
3	B	215	Total	O	0	0
			215	215		
3	C	132	Total	O	0	0
			132	132		
3	D	183	Total	O	0	0
			183	183		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	21	Total O 21 21	0	0
3	F	23	Total O 23 23	0	0
3	G	28	Total O 28 28	0	0
3	H	22	Total O 22 22	0	0

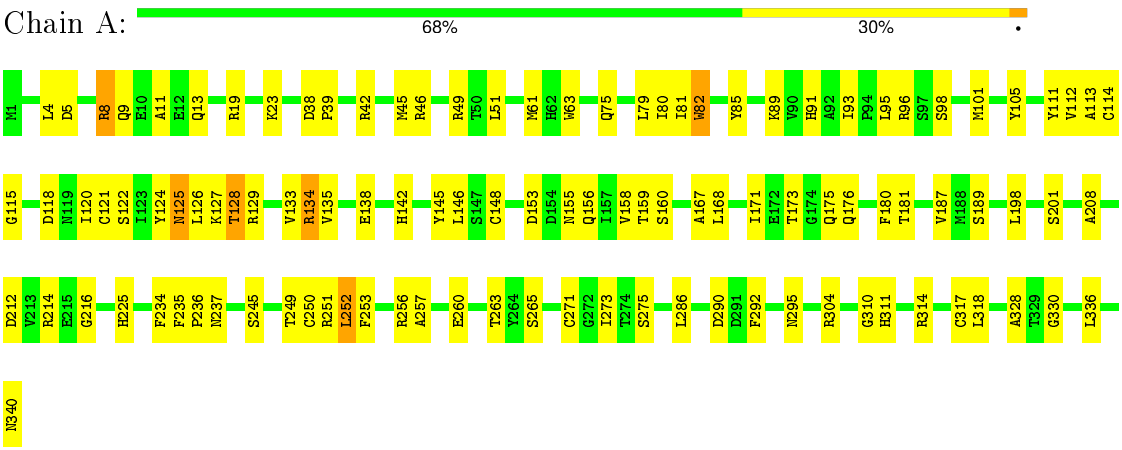
3 Residue-property plots (i)

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.

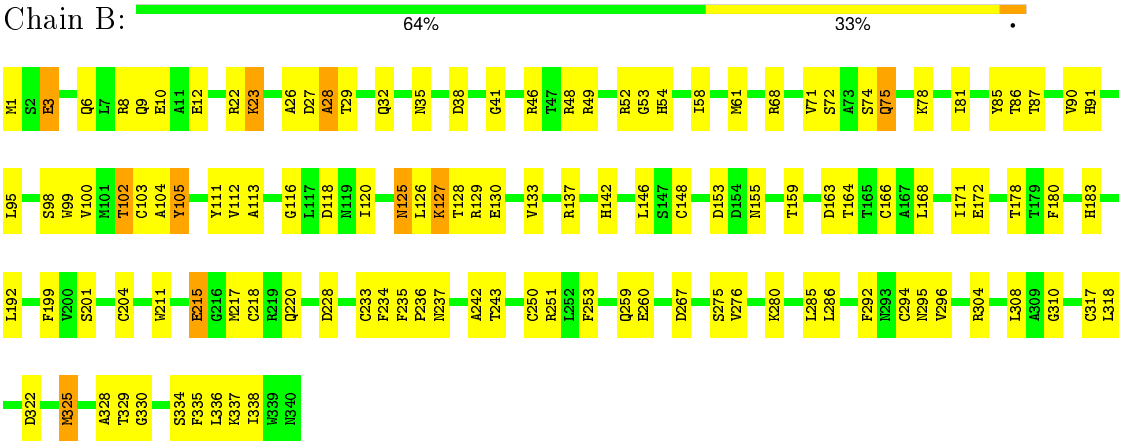
- Molecule 1: TRANSDUCIN

Chain A:



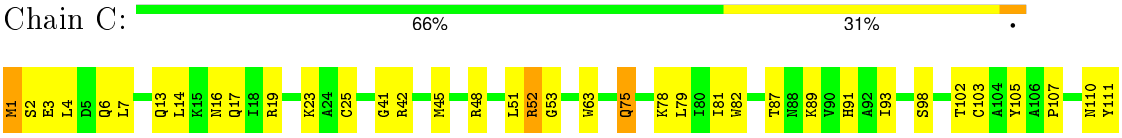
- Molecule 1: TRANSDUCIN

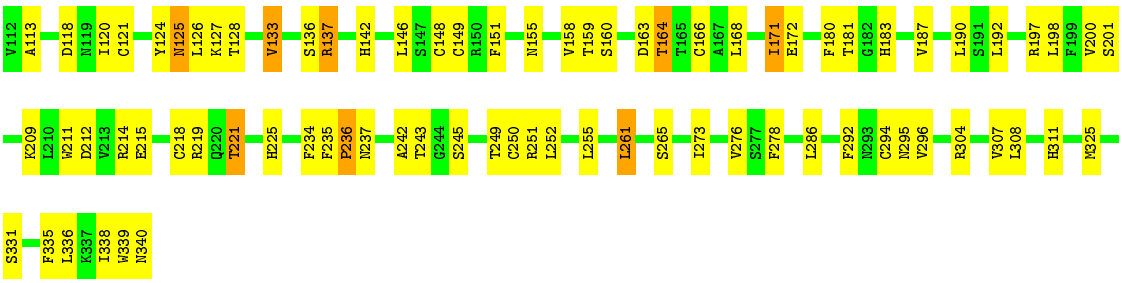
Chain B:



- Molecule 1: TRANSDUCIN

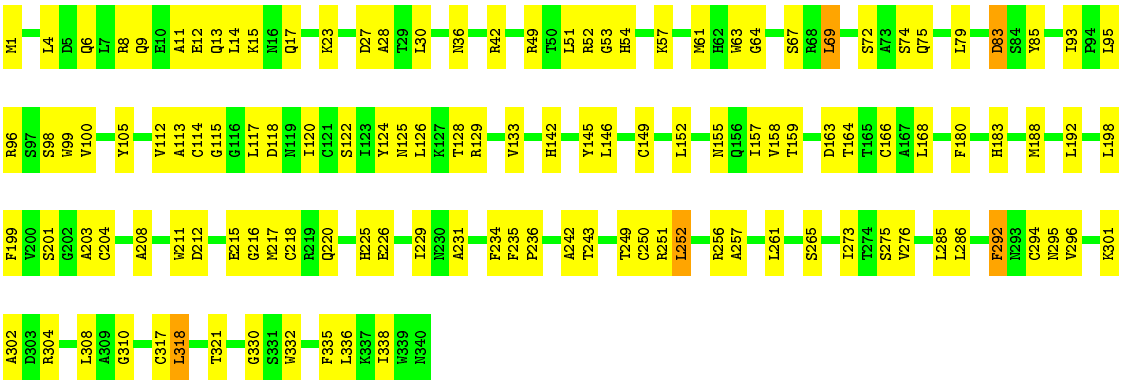
Chain C:





• Molecule 1: TRANSDUCIN

Chain D:



• Molecule 2: TRANSDUCIN

Chain E:

• Molecule 2: TRANSDUCIN

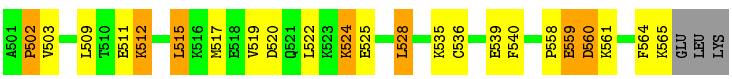
Chain F:

• Molecule 2: TRANSDUCIN

Chain G:

• Molecule 2: TRANSDUCIN

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 21	Depositor
Cell constants a, b, c, α, β, γ	85.10Å 94.00Å 194.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13273	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0/2662	0.65	0/3607
1	B	0.42	0/2662	0.75	0/3607
1	C	0.41	0/2662	0.71	0/3607
1	D	0.40	0/2662	0.73	1/3607 (0.0%)
2	E	0.41	0/529	0.59	1/708 (0.1%)
2	F	0.40	0/524	0.59	0/703
2	G	0.39	0/532	0.62	1/711 (0.1%)
2	H	0.41	0/517	0.66	1/691 (0.1%)
All	All	0.40	0/12750	0.70	4/17241 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	502	PRO	N-CA-CB	6.30	110.86	103.30
2	E	502	PRO	N-CA-CB	5.66	110.09	103.30
1	D	83	ASP	N-CA-C	-5.51	96.13	111.00
2	G	502	PRO	N-CA-CB	5.35	109.72	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2615	0	2522	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2615	0	2522	83	0
1	C	2615	0	2522	87	0
1	D	2615	0	2522	83	0
2	E	524	0	492	18	0
2	F	518	0	512	14	0
2	G	527	0	530	22	0
2	H	512	0	497	11	0
3	A	108	0	0	4	0
3	B	215	0	0	3	0
3	C	132	0	0	2	0
3	D	183	0	0	4	0
3	E	21	0	0	0	0
3	F	23	0	0	0	0
3	G	28	0	0	0	0
3	H	22	0	0	0	0
All	All	13273	0	12119	364	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 15.

All (364) 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:41:GLY:HA2	1:D:42:ARG:H	1.35	0.90
2:E:532:LEU:HB2	2:E:535:LYS:HD3	1.52	0.90
1:A:95:LEU:HD21	1:A:114:CYS:SG	2.13	0.88
2:G:512:LYS:HG2	2:G:516:LYS:HZ2	1.43	0.84
1:C:209:LYS:HG2	1:C:221:THR:HB	1.58	0.84
1:B:204:CYS:HA	1:B:228:ASP:HB3	1.61	0.82
1:B:71:VAL:HG11	1:B:112:VAL:HG11	1.62	0.81
1:C:102:THR:HG23	3:C:390:HOH:O	1.82	0.80
1:A:114:CYS:HG	1:A:124:TYR:HE1	1.31	0.78
1:C:146:LEU:HD11	1:C:159:THR:HB	1.66	0.76
1:B:204:CYS:HA	1:B:228:ASP:CB	2.15	0.76
1:A:250:CYS:SG	1:A:273:ILE:HD13	2.26	0.76
1:C:163:ASP:O	1:C:164:THR:HB	1.85	0.76
1:D:220:GLN:HG2	2:H:528:LEU:HD21	1.66	0.75
2:H:558:PRO:HG2	2:H:561:LYS:HB2	1.68	0.75
1:A:155:ASN:HA	1:A:171:ILE:HG12	1.70	0.73
1:A:180:PHE:CE1	1:A:216:GLY:HA2	2.25	0.72
1:B:183:HIS:HE1	1:B:201:SER:OG	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASP:O	1:B:164:THR:HB	1.90	0.71
1:A:51:LEU:HB2	1:A:336:LEU:HB2	1.73	0.71
1:C:4:LEU:HD21	3:D:480:HOH:O	1.90	0.70
1:B:72:SER:HB3	1:B:336:LEU:HD11	1.73	0.70
1:D:294:CYS:HB3	1:D:308:LEU:HB2	1.73	0.70
1:C:183:HIS:HE1	1:C:201:SER:OG	1.75	0.70
1:B:142:HIS:HE1	1:B:159:THR:OG1	1.75	0.70
1:B:54:HIS:O	1:B:334:SER:HB3	1.92	0.70
1:D:286:LEU:HG	1:D:296:VAL:HB	1.74	0.69
1:B:233:CYS:HB2	3:B:425:HOH:O	1.93	0.69
2:E:531:MET:HG3	2:E:535:LYS:HE2	1.74	0.69
1:B:102:THR:HG21	1:B:148:CYS:HA	1.74	0.67
2:F:565:LYS:HE2	2:F:565:LYS:HA	1.77	0.67
1:A:38:ASP:HB3	1:C:42:ARG:NH1	2.10	0.67
1:D:183:HIS:HE1	1:D:201:SER:OG	1.78	0.66
2:F:542:ASP:O	2:F:546:GLU:HG2	1.97	0.65
1:B:71:VAL:HG12	1:B:81:ILE:HG13	1.78	0.65
1:A:114:CYS:SG	1:A:124:TYR:CE1	2.90	0.65
1:D:212:ASP:HB3	1:D:215:GLU:HG2	1.78	0.65
1:D:198:LEU:HD23	1:D:212:ASP:HA	1.79	0.64
1:A:114:CYS:SG	1:A:124:TYR:HE1	2.21	0.64
1:B:178:THR:HG1	2:F:501:ALA:N	1.96	0.63
2:E:515:LEU:O	2:E:519:VAL:HG13	1.99	0.63
1:B:125:ASN:O	1:B:133:VAL:HG23	1.97	0.63
1:D:114:CYS:HG	1:D:124:TYR:HE1	1.45	0.62
2:F:525:GLU:O	2:F:528:LEU:HB2	1.99	0.62
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.64	0.62
1:C:249:THR:HG22	1:C:265:SER:HB3	1.82	0.62
2:G:512:LYS:HG2	2:G:516:LYS:NZ	2.14	0.62
2:H:520:ASP:O	2:H:524:LYS:HD2	2.00	0.62
1:D:117:LEU:HD23	1:D:145:TYR:HB3	1.81	0.61
1:C:197:ARG:HH12	1:C:219:ARG:HH22	1.48	0.61
2:F:520:ASP:O	2:F:524:LYS:HG2	2.00	0.61
1:D:180:PHE:CE1	1:D:216:GLY:HA2	2.35	0.61
1:B:118:ASP:O	1:B:120:ILE:HG12	2.00	0.60
1:B:103:CYS:HA	1:B:113:ALA:O	2.01	0.60
1:C:52:ARG:HG3	1:C:335:PHE:HE1	1.67	0.60
1:C:242:ALA:HA	1:C:251:ARG:O	2.02	0.60
1:B:86:THR:O	1:B:87:THR:HB	2.01	0.60
1:D:67:SER:HB3	1:D:321:THR:HB	1.83	0.60
2:E:555:LYS:HB2	2:E:555:LYS:NZ	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:CYS:HA	1:C:113:ALA:O	2.02	0.60
1:C:155:ASN:HA	1:C:171:ILE:HG12	1.83	0.60
1:C:198:LEU:HD23	1:C:212:ASP:HA	1.84	0.59
1:C:75:GLN:HA	1:C:98:SER:O	2.02	0.59
1:B:280:LYS:HE2	1:B:322:ASP:O	2.02	0.59
1:D:235:PHE:CD1	1:D:236:PRO:HD2	2.38	0.59
1:A:173:THR:HB	1:A:175:GLN:OE1	2.03	0.59
1:D:57:LYS:HE3	1:D:332:TRP:CD2	2.39	0.58
1:B:52:ARG:HG2	1:B:335:PHE:CE1	2.38	0.58
1:B:235:PHE:CD1	1:B:236:PRO:HD2	2.38	0.58
1:A:265:SER:HB2	3:A:404:HOH:O	2.03	0.58
1:A:198:LEU:HD23	1:A:212:ASP:HA	1.86	0.58
2:G:558:PRO:HG2	2:G:561:LYS:HB2	1.85	0.57
1:B:125:ASN:HB3	1:B:129:ARG:HE	1.67	0.57
1:D:75:GLN:O	1:D:98:SER:HB2	2.04	0.57
1:B:166:CYS:HB2	1:B:180:PHE:HB2	1.87	0.57
1:C:13:GLN:O	1:C:17:GLN:HG3	2.04	0.57
1:C:142:HIS:HE1	1:C:159:THR:OG1	1.88	0.57
1:A:112:VAL:HG23	1:A:124:TYR:HB2	1.87	0.56
1:B:49:ARG:HB2	1:B:338:ILE:HD13	1.88	0.56
1:A:63:TRP:CZ2	1:A:328:ALA:HB2	2.40	0.56
1:C:102:THR:CG2	1:C:148:CYS:HA	2.36	0.56
1:A:75:GLN:O	1:A:98:SER:HB3	2.05	0.56
1:A:167:ALA:HB1	1:A:176:GLN:HG3	1.88	0.56
2:G:519:VAL:HG12	2:G:523:LYS:HE3	1.87	0.56
1:D:257:ALA:HB2	2:H:536:CYS:SG	2.46	0.55
1:B:71:VAL:HG13	1:B:105:TYR:CE2	2.41	0.55
1:D:152:LEU:HD11	1:D:158:VAL:HG23	1.86	0.55
1:B:35:ASN:HB3	3:B:401:HOH:O	2.05	0.55
1:C:48:ARG:HH11	2:G:562:ASN:ND2	2.04	0.55
1:D:163:ASP:O	1:D:164:THR:HB	2.06	0.55
1:C:102:THR:HG21	1:C:148:CYS:HA	1.87	0.55
1:D:321:THR:HG21	3:D:410:HOH:O	2.08	0.54
1:A:96:ARG:H	1:A:96:ARG:HD2	1.71	0.54
1:B:276:VAL:HG22	1:B:285:LEU:HD11	1.89	0.54
1:A:153:ASP:OD1	1:A:156:GLN:HB2	2.07	0.54
1:A:115:GLY:HA3	1:A:146:LEU:HD23	1.89	0.54
1:D:115:GLY:HA3	1:D:146:LEU:HD23	1.89	0.54
1:A:101:MET:SD	1:A:145:TYR:CD1	3.00	0.54
1:A:135:VAL:HG21	1:A:138:GLU:HG3	1.88	0.54
1:C:110:ASN:OD1	1:C:127:LYS:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:SER:O	1:A:208:ALA:HA	2.09	0.53
1:C:82:TRP:HA	1:C:89:LYS:HA	1.89	0.53
1:D:317:CYS:SG	1:D:330:GLY:HA3	2.48	0.53
1:B:192:LEU:HD23	1:B:199:PHE:HB3	1.88	0.53
1:B:75:GLN:HA	1:B:75:GLN:HE21	1.72	0.53
1:C:243:THR:O	1:C:250:CYS:HA	2.09	0.53
1:B:23:LYS:HE2	1:B:26:ALA:HB3	1.91	0.53
1:C:160:SER:HB2	1:C:187:VAL:CG1	2.39	0.53
2:G:512:LYS:O	2:G:516:LYS:HG3	2.09	0.53
1:C:294:CYS:HB3	1:C:308:LEU:HB2	1.91	0.53
1:B:6:GLN:O	1:B:10:GLU:HB2	2.09	0.52
1:C:42:ARG:NH1	1:C:304:ARG:O	2.43	0.52
1:A:235:PHE:CD1	1:A:236:PRO:HD2	2.45	0.52
1:C:19:ARG:O	1:C:23:LYS:HG2	2.09	0.52
1:C:295:ASN:HD22	1:C:307:VAL:HG22	1.75	0.52
1:C:102:THR:HG22	1:C:103:CYS:N	2.24	0.52
1:A:275:SER:HB2	1:A:318:LEU:HG	1.92	0.52
1:A:19:ARG:HD2	1:A:23:LYS:HE3	1.91	0.52
1:B:220:GLN:HG2	2:F:528:LEU:HD21	1.92	0.52
1:B:71:VAL:CG1	1:B:81:ILE:HG13	2.40	0.52
2:G:519:VAL:O	2:G:523:LYS:HG3	2.09	0.51
1:B:27:ASP:O	1:B:28:ALA:HB2	2.10	0.51
1:B:68:ARG:HG3	1:B:85:TYR:CD1	2.45	0.51
1:D:14:LEU:HA	1:D:17:GLN:HE21	1.75	0.51
1:A:125:ASN:HD21	1:A:128:THR:N	2.08	0.51
1:D:118:ASP:O	1:D:120:ILE:HG12	2.10	0.51
2:H:559:GLU:HG2	2:H:560:ASP:H	1.74	0.51
1:D:275:SER:HB2	1:D:318:LEU:CD2	2.39	0.51
2:H:525:GLU:O	2:H:528:LEU:HB2	2.10	0.51
1:C:52:ARG:HG3	1:C:335:PHE:CE1	2.44	0.51
1:C:121:CYS:HB2	1:C:146:LEU:HD22	1.93	0.51
2:G:558:PRO:HB2	2:G:560:ASP:OD1	2.10	0.51
1:D:6:GLN:HA	1:D:9:GLN:HG2	1.93	0.51
1:A:80:ILE:HG21	1:A:89:LYS:HD2	1.93	0.51
1:B:253:PHE:HA	1:B:260:GLU:HA	1.93	0.51
1:B:295:ASN:ND2	1:B:304:ARG:HD2	2.27	0.51
1:B:81:ILE:HD12	1:B:81:ILE:N	2.26	0.50
1:A:250:CYS:SG	1:A:273:ILE:CD1	2.99	0.50
1:A:252:LEU:HD11	2:E:540:PHE:CZ	2.46	0.50
1:B:102:THR:CG2	1:B:148:CYS:HA	2.40	0.50
1:A:134:ARG:HH11	1:A:134:ARG:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:PHE:N	1:D:292:PHE:CD1	2.77	0.50
1:A:113:ALA:HA	1:A:122:SER:O	2.11	0.50
1:D:211:TRP:CZ3	1:D:218:CYS:HB2	2.46	0.50
1:D:57:LYS:HG2	1:D:332:TRP:HB3	1.91	0.50
1:A:317:CYS:SG	1:A:330:GLY:HA3	2.52	0.50
1:A:295:ASN:ND2	1:A:304:ARG:HD2	2.27	0.50
1:D:149:CYS:HB2	1:D:157:ILE:HD11	1.93	0.50
1:C:325:MET:SD	2:G:557:ILE:HD12	2.52	0.50
1:A:142:HIS:HE1	1:A:159:THR:OG1	1.95	0.50
1:D:112:VAL:HG13	1:D:126:LEU:HD11	1.93	0.50
1:C:118:ASP:O	1:C:120:ILE:HG12	2.12	0.50
2:E:521:GLN:HE21	2:E:525:GLU:HG3	1.77	0.49
1:A:9:GLN:O	1:A:13:GLN:HG3	2.12	0.49
2:H:564:PHE:O	2:H:565:LYS:HD2	2.13	0.49
1:B:41:GLY:HA2	1:D:42:ARG:N	2.15	0.49
1:B:48:ARG:NH1	2:F:565:LYS:HE3	2.27	0.49
1:D:155:ASN:HB2	3:D:503:HOH:O	2.12	0.49
1:D:276:VAL:HG13	1:D:285:LEU:HD11	1.95	0.49
1:D:49:ARG:HH12	1:D:85:TYR:HA	1.78	0.49
1:B:99:TRP:O	1:B:116:GLY:HA3	2.12	0.49
1:C:211:TRP:CZ3	1:C:218:CYS:HB2	2.47	0.49
1:D:125:ASN:ND2	1:D:129:ARG:HE	2.10	0.49
1:C:215:GLU:O	2:G:501:ALA:N	2.45	0.49
1:B:215:GLU:HG2	1:B:217:MET:H	1.77	0.48
1:D:93:ILE:HG12	1:D:133:VAL:HG11	1.96	0.48
1:C:235:PHE:CD1	1:C:236:PRO:HD2	2.48	0.48
2:E:531:MET:SD	2:E:536:CYS:SG	3.04	0.48
1:A:257:ALA:HB2	2:E:536:CYS:SG	2.53	0.48
2:G:519:VAL:CG1	2:G:523:LYS:HE3	2.43	0.48
1:A:126:LEU:HD23	1:A:133:VAL:HG21	1.94	0.48
2:E:519:VAL:O	2:E:523:LYS:HG2	2.14	0.48
1:B:127:LYS:O	1:B:129:ARG:N	2.47	0.48
1:C:107:PRO:HD3	1:C:151:PHE:HB2	1.95	0.48
1:B:72:SER:CB	1:B:336:LEU:HD11	2.42	0.48
2:G:542:ASP:O	2:G:546:GLU:HG3	2.13	0.48
1:C:125:ASN:HB2	1:C:136:SER:OG	2.13	0.48
1:D:188:MET:SD	1:D:204:CYS:SG	3.12	0.48
1:D:159:THR:O	1:D:166:CYS:HA	2.14	0.47
1:A:81:ILE:HD13	1:A:91:HIS:HB2	1.96	0.47
1:A:286:LEU:N	1:A:286:LEU:HD12	2.30	0.47
1:B:61:MET:HA	1:B:71:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:HA	1:A:328:ALA:O	2.14	0.47
1:A:81:ILE:HB	1:A:91:HIS:HB2	1.95	0.47
1:B:325:MET:HG3	2:F:557:ILE:HD13	1.95	0.47
1:D:11:ALA:O	1:D:15:LYS:HG3	2.14	0.47
1:D:8:ARG:HG3	2:H:515:LEU:HD11	1.96	0.47
1:C:102:THR:HG21	1:C:149:CYS:N	2.30	0.47
1:D:188:MET:HB2	1:D:229:ILE:O	2.14	0.47
1:D:192:LEU:HD23	1:D:199:PHE:HB3	1.96	0.47
1:C:252:LEU:HD23	1:C:278:PHE:HZ	1.80	0.47
1:A:225:HIS:HA	1:A:251:ARG:NH1	2.29	0.47
1:C:14:LEU:HD13	2:G:522:LEU:HB3	1.97	0.47
1:A:42:ARG:N	1:C:41:GLY:HA2	2.29	0.47
2:F:523:LYS:O	2:F:526:VAL:HG12	2.14	0.47
1:D:13:GLN:O	1:D:17:GLN:HG3	2.15	0.47
1:B:215:GLU:OE2	1:B:217:MET:HB2	2.15	0.47
1:A:49:ARG:HG3	1:A:49:ARG:NH1	2.30	0.47
1:A:38:ASP:HB3	1:C:42:ARG:HH12	1.81	0.46
1:C:125:ASN:O	1:C:133:VAL:HG23	2.14	0.46
2:G:518:GLU:HG2	2:G:522:LEU:HD22	1.97	0.46
1:B:155:ASN:OD1	1:B:172:GLU:HB2	2.15	0.46
2:F:510:THR:H	2:F:513:ASP:HB2	1.79	0.46
1:A:118:ASP:O	1:A:120:ILE:HG13	2.15	0.46
1:A:39:PRO:O	1:C:42:ARG:HD3	2.15	0.46
1:C:160:SER:HB2	1:C:187:VAL:HG11	1.96	0.46
1:A:160:SER:HB2	1:A:187:VAL:CG1	2.45	0.46
1:B:8:ARG:O	1:B:12:GLU:HG2	2.15	0.46
1:B:48:ARG:HH11	2:F:565:LYS:HE3	1.81	0.46
1:A:148:CYS:HB3	1:A:189:SER:HA	1.96	0.46
1:C:166:CYS:HB2	1:C:180:PHE:HB2	1.97	0.46
1:A:45:MET:SD	2:E:553:LEU:HD22	2.56	0.46
2:F:552:PRO:HB3	2:F:557:ILE:HD11	1.98	0.46
1:B:317:CYS:SG	1:B:330:GLY:HA3	2.56	0.46
1:D:180:PHE:HE1	1:D:216:GLY:HA2	1.77	0.45
1:D:52:ARG:HG2	1:D:335:PHE:CD1	2.50	0.45
1:B:75:GLN:HA	1:B:98:SER:O	2.16	0.45
1:D:275:SER:HB2	1:D:318:LEU:HD22	1.99	0.45
1:B:275:SER:HB2	1:B:318:LEU:HG	1.97	0.45
1:A:111:TYR:HA	1:A:124:TYR:O	2.17	0.45
1:A:128:THR:O	1:A:128:THR:HG22	2.17	0.45
1:D:8:ARG:O	1:D:12:GLU:HG2	2.16	0.45
1:A:225:HIS:CE1	1:A:245:SER:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:HA	1:B:328:ALA:O	2.17	0.45
1:A:263:THR:HG21	3:A:415:HOH:O	2.17	0.45
1:A:80:ILE:CG2	1:A:89:LYS:HD2	2.47	0.45
1:D:51:LEU:HB2	1:D:336:LEU:HB2	1.98	0.45
1:B:164:THR:HG23	1:B:183:HIS:O	2.17	0.45
1:B:295:ASN:HD22	1:B:304:ARG:HD2	1.82	0.45
1:C:235:PHE:CG	1:C:236:PRO:HD2	2.52	0.45
1:C:87:THR:O	1:C:87:THR:HG22	2.16	0.45
1:B:292:PHE:CD1	1:B:292:PHE:N	2.84	0.45
1:B:294:CYS:HB3	1:B:308:LEU:HB2	1.98	0.45
1:D:201:SER:O	1:D:208:ALA:HA	2.16	0.45
2:G:549:GLY:O	2:G:555:LYS:HD3	2.17	0.45
2:E:508:ASP:C	2:E:509:LEU:HD22	2.37	0.45
1:A:292:PHE:HB3	1:A:311:HIS:O	2.17	0.45
1:A:61:MET:HE1	1:A:328:ALA:HB3	2.00	0.44
1:B:328:ALA:HA	1:B:337:LYS:O	2.17	0.44
1:A:63:TRP:HZ2	1:A:328:ALA:HB2	1.80	0.44
1:C:79:LEU:HB3	1:C:93:ILE:HB	1.98	0.44
1:C:249:THR:OG1	1:C:251:ARG:NH1	2.51	0.44
1:A:158:VAL:HA	1:A:167:ALA:O	2.17	0.44
1:C:48:ARG:HH11	2:G:562:ASN:HD21	1.65	0.44
1:A:225:HIS:ND1	1:A:251:ARG:NH1	2.61	0.44
1:D:249:THR:HG22	1:D:265:SER:HB3	1.98	0.44
1:C:295:ASN:ND2	1:C:307:VAL:HG22	2.33	0.44
1:C:252:LEU:HD12	1:C:261:LEU:HD22	2.00	0.44
1:A:79:LEU:HB3	1:A:93:ILE:HB	1.99	0.44
2:H:535:LYS:O	2:H:539:GLU:HG3	2.17	0.44
1:D:183:HIS:CD2	1:D:203:ALA:HB3	2.53	0.44
1:B:294:CYS:SG	1:B:308:LEU:HD12	2.57	0.44
1:D:243:THR:O	1:D:250:CYS:HA	2.18	0.44
1:C:158:VAL:HG11	1:C:192:LEU:HD21	1.99	0.44
1:D:67:SER:CB	1:D:321:THR:HB	2.46	0.44
1:D:225:HIS:CE1	1:D:251:ARG:HH11	2.35	0.44
1:D:301:LYS:O	1:D:302:ALA:HB3	2.18	0.44
1:B:104:ALA:O	1:B:112:VAL:HA	2.18	0.44
1:A:235:PHE:HD2	1:A:237:ASN:OD1	2.01	0.44
1:A:79:LEU:HD22	1:A:114:CYS:SG	2.58	0.43
1:C:218:CYS:SG	2:G:521:GLN:NE2	2.91	0.43
1:A:225:HIS:HE1	1:A:249:THR:O	2.01	0.43
1:B:22:ARG:HG2	1:B:259:GLN:HB3	2.00	0.43
1:C:308:LEU:HD22	1:C:339:TRP:CE3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:THR:OG1	1:D:251:ARG:NH1	2.51	0.43
1:C:1:MET:N	1:C:6:GLN:OE1	2.51	0.43
1:D:57:LYS:HG2	1:D:332:TRP:CB	2.48	0.43
1:C:48:ARG:NH1	2:G:562:ASN:ND2	2.66	0.43
1:C:235:PHE:HD2	1:C:237:ASN:OD1	2.01	0.43
1:D:79:LEU:HD13	1:D:95:LEU:HD21	2.00	0.43
1:C:164:THR:HG23	1:C:183:HIS:O	2.18	0.43
1:D:142:HIS:HE1	1:D:159:THR:OG1	2.02	0.43
1:C:211:TRP:CE3	1:C:218:CYS:HB2	2.54	0.43
1:B:338:ILE:N	1:B:338:ILE:HD12	2.33	0.43
1:A:120:ILE:HG22	1:A:121:CYS:N	2.34	0.43
1:B:242:ALA:HA	1:B:251:ARG:O	2.18	0.43
1:A:290:ASP:HA	1:A:314:ARG:HG3	1.99	0.43
1:C:53:GLY:HA3	1:C:89:LYS:NZ	2.33	0.43
1:B:102:THR:HG22	1:B:103:CYS:H	1.82	0.43
1:D:69:LEU:HD12	1:D:83:ASP:HA	2.01	0.43
1:A:4:LEU:HD21	1:A:8:ARG:HH21	1.83	0.43
1:B:3:GLU:O	1:B:6:GLN:HG2	2.19	0.43
1:B:233:CYS:SG	1:B:276:VAL:HG13	2.59	0.42
1:C:75:GLN:O	1:C:98:SER:HB2	2.19	0.42
1:D:142:HIS:HD2	1:D:163:ASP:OD2	2.03	0.42
1:D:242:ALA:HA	1:D:251:ARG:O	2.19	0.42
1:D:54:HIS:CG	1:D:74:SER:HG	2.34	0.42
1:B:29:THR:OG1	1:B:32:GLN:HG3	2.19	0.42
1:C:51:LEU:HB2	1:C:336:LEU:HB2	2.01	0.42
1:D:114:CYS:SG	1:D:124:TYR:HE1	2.42	0.42
1:D:113:ALA:HA	1:D:122:SER:O	2.19	0.42
1:B:111:TYR:CD2	1:B:125:ASN:HA	2.54	0.42
1:C:252:LEU:CD2	1:C:278:PHE:HZ	2.32	0.42
1:B:211:TRP:CZ3	1:B:218:CYS:HB2	2.55	0.42
1:D:215:GLU:OE1	1:D:217:MET:SD	2.77	0.42
1:C:155:ASN:OD1	1:C:172:GLU:HB2	2.20	0.42
1:C:137:ARG:HB2	3:C:466:HOH:O	2.19	0.42
1:D:30:LEU:HD21	2:H:540:PHE:CD2	2.54	0.42
1:D:235:PHE:CG	1:D:236:PRO:HD2	2.54	0.42
1:D:75:GLN:NE2	1:D:99:TRP:HA	2.34	0.42
1:D:72:SER:HB2	1:D:336:LEU:HD11	2.02	0.42
1:B:243:THR:O	1:B:250:CYS:HA	2.20	0.42
1:D:23:LYS:HE3	1:D:23:LYS:HB2	1.85	0.42
1:A:125:ASN:OD1	1:A:128:THR:HB	2.19	0.42
1:B:237:ASN:HB3	2:F:543:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:GLY:HA2	3:D:412:HOH:O	2.20	0.42
1:A:82:TRP:CD1	1:A:82:TRP:N	2.87	0.42
1:D:27:ASP:O	1:D:28:ALA:HB2	2.20	0.42
1:A:127:LYS:C	1:A:129:ARG:H	2.23	0.42
1:D:125:ASN:HD22	1:D:129:ARG:HE	1.66	0.42
1:A:181:THR:OG1	2:E:501:ALA:HA	2.20	0.42
1:D:295:ASN:ND2	1:D:304:ARG:HH11	2.17	0.42
1:D:146:LEU:CD1	1:D:159:THR:HB	2.50	0.42
1:C:339:TRP:O	1:C:340:ASN:HB3	2.20	0.42
2:F:560:ASP:OD1	2:F:561:LYS:HG2	2.20	0.42
1:B:329:THR:O	1:B:336:LEU:HA	2.20	0.41
1:C:25:CYS:HA	2:G:532:LEU:HD23	2.02	0.41
2:E:550:GLU:O	2:E:552:PRO:HD3	2.19	0.41
1:B:90:VAL:O	1:B:91:HIS:ND1	2.53	0.41
1:C:273:ILE:N	1:C:273:ILE:HD12	2.34	0.41
1:C:4:LEU:N	1:C:4:LEU:HD22	2.35	0.41
1:C:325:MET:SD	2:G:557:ILE:CD1	3.08	0.41
1:A:5:ASP:HB2	3:B:543:HOH:O	2.21	0.41
1:C:286:LEU:N	1:C:286:LEU:HD12	2.36	0.41
1:D:273:ILE:N	1:D:273:ILE:HD12	2.35	0.41
1:C:111:TYR:HD1	1:C:124:TYR:O	2.03	0.41
1:D:125:ASN:O	1:D:133:VAL:HG23	2.19	0.41
1:A:189:SER:HB3	3:A:362:HOH:O	2.20	0.41
1:D:4:LEU:HD23	2:H:512:LYS:HD3	2.02	0.41
1:C:311:HIS:ND1	1:C:331:SER:HB3	2.35	0.41
1:B:81:ILE:HD13	1:B:91:HIS:HB2	2.02	0.41
1:B:146:LEU:HD11	1:B:159:THR:HB	2.01	0.41
1:C:48:ARG:HD3	1:C:48:ARG:HA	1.82	0.41
1:C:78:LYS:HB2	1:C:78:LYS:HE2	1.83	0.41
1:B:286:LEU:N	1:B:286:LEU:HD12	2.35	0.41
1:A:11:ALA:HB2	2:E:519:VAL:HG12	2.02	0.41
1:A:49:ARG:NH1	1:A:85:TYR:O	2.54	0.41
1:D:149:CYS:HA	1:D:158:VAL:O	2.20	0.41
1:C:45:MET:HB2	1:C:308:LEU:HD21	2.03	0.41
2:E:510:THR:C	2:E:512:LYS:H	2.24	0.41
1:B:54:HIS:CG	1:B:74:SER:HB3	2.56	0.41
1:A:271:CYS:HB2	1:A:290:ASP:HB2	2.02	0.41
2:E:510:THR:O	2:E:514:LYS:HE3	2.20	0.41
1:D:252:LEU:HD13	1:D:261:LEU:HB2	2.02	0.41
1:C:63:TRP:CH2	1:C:338:ILE:HD12	2.56	0.41
1:B:58:ILE:HD13	1:B:336:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:HD21	1:A:129:ARG:N	2.19	0.41
1:A:5:ASP:HB3	3:A:411:HOH:O	2.19	0.41
1:D:63:TRP:CH2	1:D:338:ILE:HD12	2.56	0.41
1:C:181:THR:CG2	2:G:506:ILE:HD11	2.51	0.41
1:C:81:ILE:HD13	1:C:91:HIS:HB2	2.03	0.40
1:C:7:LEU:CD1	2:G:516:LYS:HG2	2.51	0.40
1:C:16:ASN:OD1	1:C:19:ARG:NH2	2.55	0.40
1:C:225:HIS:CE1	1:C:245:SER:HB3	2.56	0.40
1:B:54:HIS:ND1	1:B:74:SER:OG	2.47	0.40
1:D:231:ALA:HB2	1:D:275:SER:HA	2.03	0.40
2:E:501:ALA:N	2:E:506:ILE:O	2.55	0.40
1:B:204:CYS:HA	1:B:228:ASP:HB2	1.97	0.40
2:E:555:LYS:HZ3	2:E:555:LYS:HB2	1.85	0.40
1:A:253:PHE:HA	1:A:260:GLU:HA	2.03	0.40
1:C:292:PHE:N	1:C:292:PHE:CD1	2.88	0.40
1:B:267:ASP:H	1:D:36:ASN:HD21	1.69	0.40
1:B:126:LEU:HD23	1:B:133:VAL:HG21	2.04	0.40
1:C:190:LEU:HA	1:C:200:VAL:O	2.21	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	338/340 (99%)	309 (91%)	27 (8%)	2 (1%)	30 24
1	B	338/340 (99%)	312 (92%)	20 (6%)	6 (2%)	11 5
1	C	338/340 (99%)	313 (93%)	21 (6%)	4 (1%)	16 10
1	D	338/340 (99%)	314 (93%)	21 (6%)	3 (1%)	21 15
2	E	66/68 (97%)	50 (76%)	15 (23%)	1 (2%)	13 7
2	F	63/68 (93%)	62 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	G	63/68 (93%)	57 (90%)	4 (6%)	2 (3%)	5 1
2	H	63/68 (93%)	57 (90%)	3 (5%)	3 (5%)	3 0
All	All	1607/1632 (98%)	1474 (92%)	112 (7%)	21 (1%)	15 9

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	LYS
1	B	128	THR
2	H	502	PRO
2	H	503	VAL
1	B	3	GLU
1	C	2	SER
1	C	3	GLU
2	G	502	PRO
2	G	560	ASP
1	D	128	THR
1	A	128	THR
2	E	511	GLU
1	C	128	THR
1	B	28	ALA
1	B	310	GLY
1	D	310	GLY
2	H	559	GLU
1	A	310	GLY
1	B	53	GLY
1	C	133	VAL
1	D	53	GLY

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	283/283 (100%)	271 (96%)	12 (4%)	36 35
1	B	283/283 (100%)	262 (93%)	21 (7%)	17 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	283/283 (100%)	265 (94%)	18 (6%)	22 18
1	D	283/283 (100%)	270 (95%)	13 (5%)	33 31
2	E	55/65 (85%)	49 (89%)	6 (11%)	8 4
2	F	59/65 (91%)	51 (86%)	8 (14%)	5 2
2	G	61/65 (94%)	57 (93%)	4 (7%)	21 17
2	H	56/65 (86%)	46 (82%)	10 (18%)	2 1
All	All	1363/1392 (98%)	1271 (93%)	92 (7%)	20 16

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	46	ARG
1	A	82	TRP
1	A	105	TYR
1	A	125	ASN
1	A	134	ARG
1	A	168	LEU
1	A	214	ARG
1	A	234	PHE
1	A	252	LEU
1	A	256	ARG
1	A	340	ASN
2	E	515	LEU
2	E	522	LEU
2	E	527	THR
2	E	529	GLU
2	E	550	GLU
2	E	555	LYS
1	B	1	MET
1	B	9	GLN
1	B	23	LYS
1	B	38	ASP
1	B	46	ARG
1	B	75	GLN
1	B	78	LYS
1	B	95	LEU
1	B	100	VAL
1	B	102	THR
1	B	105	TYR

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Mol	Chain	Res	Type
1	B	125	ASN
1	B	130	GLU
1	B	137	ARG
1	B	153	ASP
1	B	168	LEU
1	B	171	ILE
1	B	215	GLU
1	B	234	PHE
1	B	296	VAL
1	B	325	MET
2	F	511	GLU
2	F	522	LEU
2	F	528	LEU
2	F	546	GLU
2	F	547	ARG
2	F	559	GLU
2	F	560	ASP
2	F	565	LYS
1	C	1	MET
1	C	52	ARG
1	C	75	GLN
1	C	105	TYR
1	C	125	ASN
1	C	126	LEU
1	C	137	ARG
1	C	164	THR
1	C	168	LEU
1	C	171	ILE
1	C	214	ARG
1	C	221	THR
1	C	234	PHE
1	C	236	PRO
1	C	255	LEU
1	C	261	LEU
1	C	276	VAL
1	C	296	VAL
2	G	503	VAL
2	G	511	GLU
2	G	522	LEU
2	G	559	GLU
1	D	1	MET
1	D	61	MET

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Mol	Chain	Res	Type
1	D	69	LEU
1	D	96	ARG
1	D	100	VAL
1	D	105	TYR
1	D	168	LEU
1	D	226	GLU
1	D	234	PHE
1	D	252	LEU
1	D	256	ARG
1	D	292	PHE
1	D	318	LEU
2	H	509	LEU
2	H	511	GLU
2	H	512	LYS
2	H	515	LEU
2	H	517	MET
2	H	519	VAL
2	H	522	LEU
2	H	524	LYS
2	H	528	LEU
2	H	560	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	125	ASN
1	A	142	HIS
1	A	183	HIS
1	A	295	ASN
2	E	521	GLN
1	B	9	GLN
1	B	75	GLN
1	B	142	HIS
1	B	176	GLN
1	B	183	HIS
1	B	220	GLN
1	B	293	ASN
1	B	295	ASN
1	C	13	GLN
1	C	17	GLN
1	C	75	GLN

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Mol	Chain	Res	Type
1	C	125	ASN
1	C	142	HIS
1	C	175	GLN
1	C	176	GLN
1	C	183	HIS
1	C	220	GLN
1	C	239	ASN
1	C	295	ASN
2	G	521	GLN
1	D	6	GLN
1	D	17	GLN
1	D	36	ASN
1	D	75	GLN
1	D	88	ASN
1	D	142	HIS
1	D	176	GLN
1	D	183	HIS
1	D	220	GLN
1	D	230	ASN
1	D	295	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.