



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:57 AM GMT

PDB ID : 3CST  
Title : Crystal structure of PI3K p110gamma catalytical domain in complex with organoruthenium inhibitor E5E2  
Authors : Xie, P.; Marmorstein, R.  
Deposited on : 2008-04-10  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

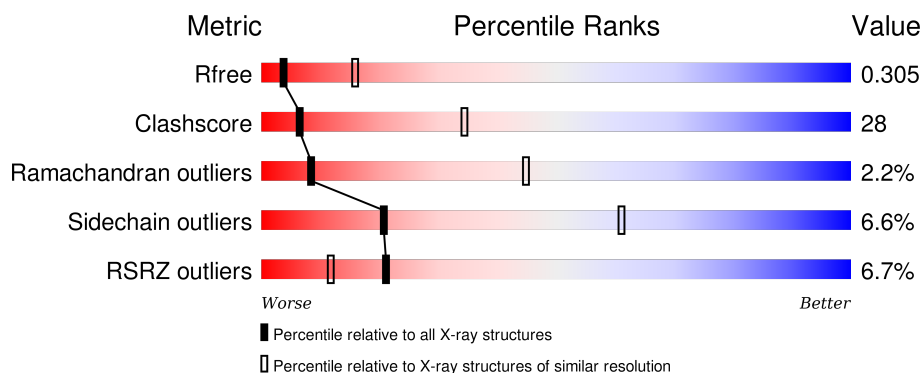
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	966	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6824 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.

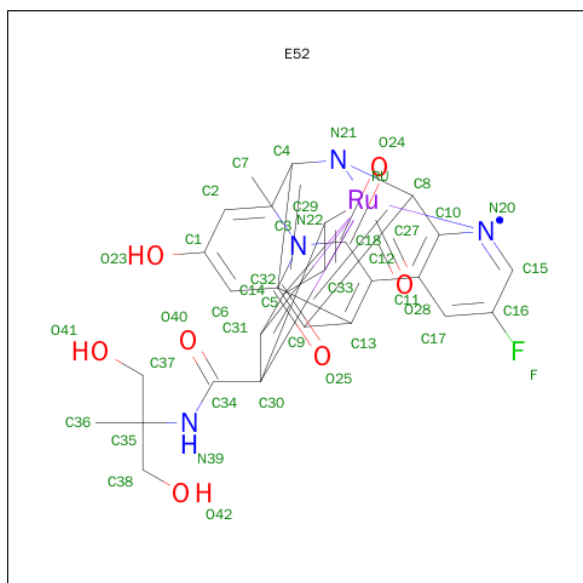
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	0	0
			6782	4350	1157	1239	36			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is METHYLATED RUTHENIUM PYRIDOCARBAZOLE (three-letter code: E52) (formula: C<sub>29</sub>H<sub>23</sub>FN<sub>4</sub>O<sub>7</sub>Ru).

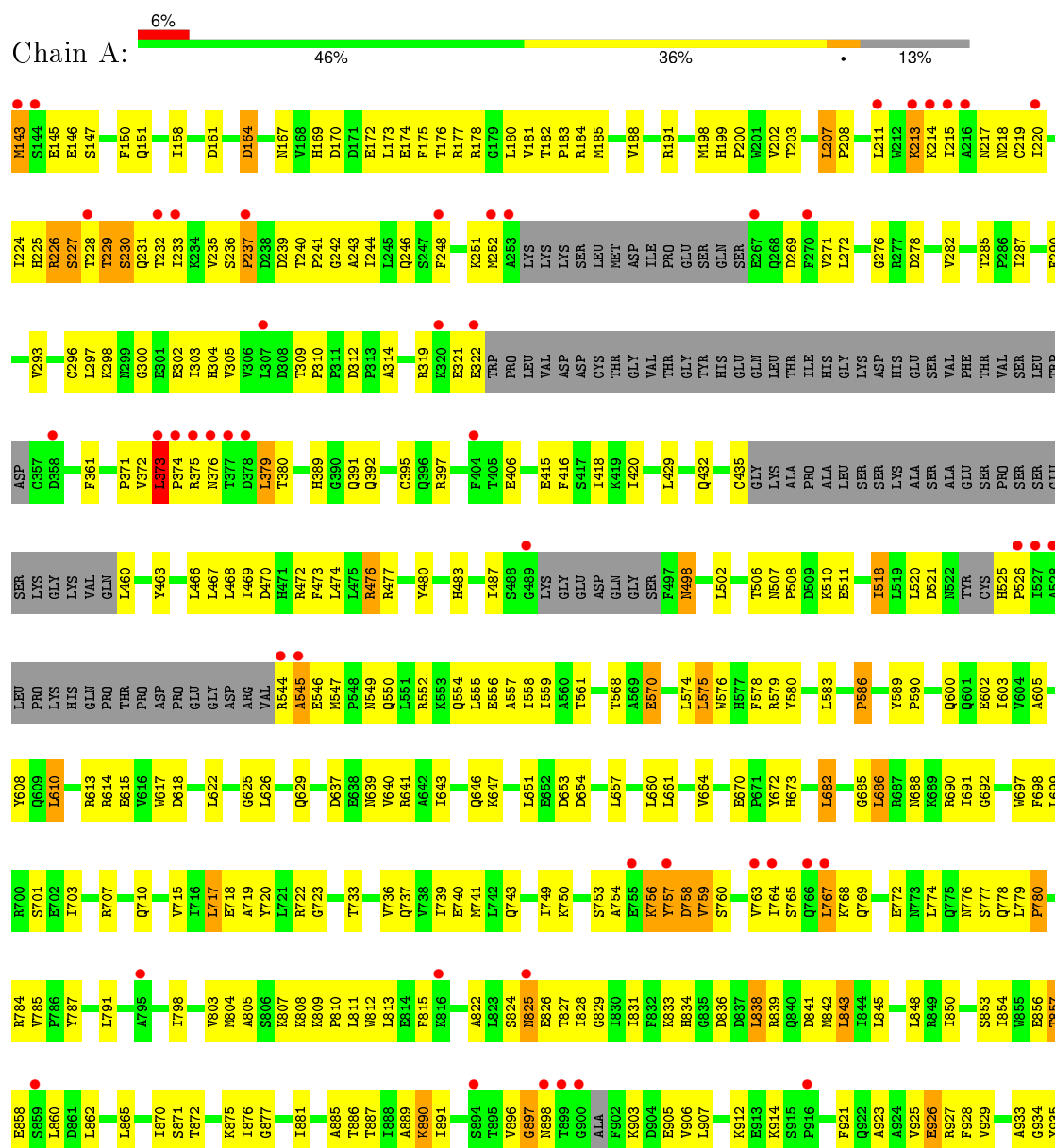


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	Ru	0	0
			42	29	1	4	7	1		

### 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.

- Molecule 1: Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.11Å 68.32Å 107.03Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 31.32 – 3.11	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-3.20) 94.0 (31.32-3.11)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.264 , 0.305 0.263 , 0.305	Depositor DCC
$R_{free}$ test set	1706 reflections (11.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 42.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 18708 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: E52

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	0.54	0/6926	0.75	2/9365 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	575	LEU	CA-CB-CG	6.05	129.21	115.30
1	A	686	LEU	CB-CG-CD2	-5.38	101.86	111.00

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	6782	0	6811	376	0
2	A	42	0	19	20	0
All	All	6824	0	6830	376	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 28.

All (376) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:LYS:HD3	2:A:1:E52:O42	1.43	1.17
1:A:890:LYS:CE	2:A:1:E52:H38A	1.77	1.14
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.30	1.14
1:A:544:ARG:HH21	1:A:546:GLU:HB3	1.13	1.10
1:A:890:LYS:HE2	2:A:1:E52:H38A	1.33	1.06
1:A:805:ALA:O	2:A:1:E52:H37A	1.56	1.05
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.33	1.04
1:A:805:ALA:HB3	2:A:1:E52:H36A	1.42	0.99
1:A:373:LEU:HD22	1:A:406:GLU:HG2	1.41	0.98
1:A:224:ILE:HD12	1:A:233:ILE:HD13	1.48	0.96
1:A:890:LYS:CD	2:A:1:E52:O42	2.24	0.86
1:A:890:LYS:NZ	2:A:1:E52:H38A	1.90	0.85
1:A:554:GLN:O	1:A:558:ILE:HD13	1.76	0.85
1:A:143:MET:HG2	1:A:147:SER:OG	1.76	0.84
1:A:207:LEU:HD23	1:A:208:PRO:HD2	1.60	0.84
1:A:896:VAL:HG12	1:A:897:GLY:H	1.40	0.84
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.25	0.83
1:A:474:LEU:HD23	1:A:525:HIS:N	1.93	0.82
1:A:890:LYS:HD2	2:A:1:E52:O28	1.78	0.82
1:A:544:ARG:NH2	1:A:546:GLU:HB3	1.92	0.82
1:A:217:ASN:HD22	1:A:219:CYS:HB2	1.45	0.82
1:A:890:LYS:CE	2:A:1:E52:C38	2.57	0.81
1:A:1060:ASN:HD21	1:A:1062:GLU:HB2	1.45	0.81
1:A:240:THR:O	1:A:244:ILE:HG23	1.81	0.80
1:A:741:MET:HE1	1:A:778:GLN:HB3	1.62	0.80
1:A:379:LEU:HD13	1:A:380:THR:H	1.46	0.79
1:A:1002:THR:HG22	1:A:1003:SER:H	1.48	0.79
1:A:217:ASN:ND2	1:A:219:CYS:HB2	1.97	0.78
1:A:768:LYS:O	1:A:772:GLU:HG2	1.84	0.78
1:A:733:THR:O	1:A:737:GLN:HG3	1.85	0.77
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.67	0.76
1:A:395:CYS:SG	1:A:418:ILE:HG13	2.25	0.76
1:A:839:ARG:HA	1:A:842:MET:HE2	1.66	0.76
1:A:824:SER:OG	1:A:826:GLU:HG3	1.85	0.75
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.69	0.75
1:A:885:ALA:O	2:A:1:E52:C2	2.34	0.75
1:A:890:LYS:HE2	2:A:1:E52:C38	2.12	0.75
1:A:1042:LEU:HD23	1:A:1048:ILE:HD11	1.68	0.74
1:A:568:THR:HG22	1:A:570:GLU:H	1.51	0.74
1:A:167:ASN:ND2	1:A:506:THR:O	2.20	0.74
1:A:812:TRP:O	1:A:812:TRP:CD1	2.41	0.74
1:A:231:GLN:HG3	1:A:232:THR:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:NH2	1:A:963:ILE:O	2.22	0.73
1:A:233:ILE:HD12	1:A:233:ILE:H	1.55	0.72
1:A:839:ARG:HA	1:A:842:MET:CE	2.19	0.71
1:A:885:ALA:N	2:A:1:E52:O23	2.22	0.71
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.72	0.71
1:A:198:MET:SD	1:A:282:VAL:HG11	2.31	0.71
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.72	0.71
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.05	0.71
1:A:833:LYS:O	1:A:876:ILE:HD12	1.90	0.71
1:A:373:LEU:CD2	1:A:406:GLU:HG2	2.20	0.70
1:A:750:LYS:HE3	1:A:809:LYS:H	1.55	0.70
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.09	0.70
1:A:463:TYR:HD2	1:A:487:ILE:HD11	1.57	0.69
1:A:180:LEU:O	1:A:183:PRO:HD2	1.92	0.69
1:A:1020:LEU:HD22	1:A:1027:LEU:HD11	1.74	0.69
1:A:765:SER:O	1:A:769:GLN:HG3	1.93	0.68
1:A:576:TRP:O	1:A:579:ARG:HD3	1.94	0.68
1:A:887:THR:HG22	1:A:889:ALA:H	1.59	0.68
1:A:758:ASP:OD1	1:A:759:VAL:N	2.26	0.68
1:A:207:LEU:CD2	1:A:208:PRO:HD2	2.24	0.68
1:A:251:LYS:HD3	1:A:251:LYS:O	1.94	0.67
1:A:1056:THR:O	1:A:1056:THR:HG23	1.95	0.67
1:A:576:TRP:CZ3	1:A:579:ARG:HD2	2.30	0.67
1:A:372:VAL:HG12	1:A:374:PRO:HD2	1.77	0.67
1:A:657:LEU:HD11	1:A:690:ARG:HD3	1.76	0.67
1:A:1043:THR:C	1:A:1045:LYS:H	1.97	0.67
1:A:580:TYR:HE2	1:A:613:ARG:HD3	1.60	0.67
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.60	0.66
1:A:805:ALA:O	2:A:1:E52:C37	2.41	0.66
1:A:812:TRP:O	1:A:812:TRP:HD1	1.76	0.66
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.17	0.66
1:A:661:LEU:HD21	1:A:843:LEU:HD13	1.76	0.66
1:A:483:HIS:CD2	1:A:510:LYS:HG3	2.30	0.66
1:A:811:LEU:HB3	1:A:813:LEU:HD21	1.78	0.66
1:A:544:ARG:HH21	1:A:546:GLU:CB	2.00	0.66
1:A:997:THR:HG22	1:A:998:SER:N	2.11	0.66
1:A:1008:LYS:O	1:A:1012:ILE:HG13	1.97	0.65
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.78	0.65
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.27	0.65
1:A:213:LYS:HD3	1:A:214:LYS:N	2.12	0.65
1:A:1043:THR:O	1:A:1045:LYS:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG12	1:A:717:LEU:HD13	1.78	0.64
1:A:568:THR:HG22	1:A:570:GLU:N	2.11	0.64
1:A:885:ALA:O	2:A:1:E52:C1	2.45	0.64
1:A:379:LEU:CD1	1:A:380:THR:H	2.10	0.64
1:A:240:THR:HG22	1:A:242:GLY:H	1.63	0.64
1:A:373:LEU:N	1:A:374:PRO:HD2	2.14	0.63
1:A:1002:THR:HG22	1:A:1003:SER:N	2.14	0.63
1:A:860:LEU:HD11	1:A:1015:LYS:HG2	1.79	0.63
1:A:660:LEU:O	1:A:664:VAL:HG23	1.99	0.63
1:A:890:LYS:HZ3	2:A:1:E52:H38A	1.61	0.63
1:A:184:ARG:HH11	1:A:184:ARG:HB2	1.63	0.62
1:A:736:VAL:O	1:A:740:GLU:HB2	1.99	0.62
1:A:525:HIS:HB3	1:A:526:PRO:CD	2.19	0.62
1:A:467:LEU:O	1:A:476:ARG:HD2	2.00	0.62
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.13	0.62
1:A:640:VAL:O	1:A:643:ILE:HG12	2.00	0.62
1:A:1000:LYS:HA	1:A:1076:ARG:NH1	2.15	0.62
1:A:576:TRP:CE3	1:A:579:ARG:HD2	2.35	0.62
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.35	0.62
1:A:896:VAL:CG2	1:A:903:LYS:HG3	2.30	0.61
1:A:1000:LYS:HA	1:A:1076:ARG:CZ	2.31	0.61
1:A:182:THR:HB	1:A:183:PRO:HD3	1.82	0.61
1:A:468:LEU:C	1:A:469:ILE:HD12	2.19	0.61
1:A:876:ILE:HG13	1:A:877:GLY:N	2.15	0.61
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.13	0.61
1:A:1009:PHE:HE2	1:A:1072:ILE:HD12	1.65	0.60
1:A:576:TRP:CH2	1:A:579:ARG:HD2	2.36	0.60
1:A:1042:LEU:O	1:A:1042:LEU:HD13	2.02	0.60
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.32	0.60
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.01	0.60
1:A:188:VAL:O	1:A:191:ARG:HG2	2.02	0.59
1:A:829:GLY:C	1:A:881:ILE:HD12	2.22	0.59
1:A:147:SER:HA	1:A:319:ARG:NH2	2.18	0.59
1:A:887:THR:HG22	1:A:889:ALA:N	2.17	0.59
1:A:278:ASP:OD1	1:A:784:ARG:NH2	2.35	0.59
1:A:583:LEU:CD1	1:A:610:LEU:HD22	2.33	0.59
1:A:804:MET:HE1	1:A:831:ILE:HD12	1.84	0.58
1:A:379:LEU:HB3	1:A:435:CYS:SG	2.43	0.58
1:A:1052:ARG:HH11	1:A:1052:ARG:HG2	1.68	0.58
1:A:779:LEU:HD23	1:A:780:PRO:O	2.03	0.58
1:A:760:SER:O	1:A:763:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ILE:N	1:A:469:ILE:HD12	2.18	0.57
1:A:583:LEU:HD12	1:A:610:LEU:HD22	1.86	0.57
1:A:1042:LEU:CD1	1:A:1042:LEU:H	2.17	0.57
1:A:890:LYS:HD3	2:A:1:E52:C38	2.34	0.57
1:A:739:ILE:O	1:A:743:GLN:HG3	2.05	0.57
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.03	0.57
1:A:220:ILE:HD11	1:A:237:PRO:HG3	1.86	0.57
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.70	0.56
1:A:935:TYR:O	1:A:939:THR:HB	2.05	0.56
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.87	0.56
1:A:1000:LYS:HG2	1:A:1076:ARG:HB3	1.86	0.56
1:A:296:CYS:SG	1:A:303:ILE:HD13	2.46	0.56
1:A:1029:ILE:O	1:A:1033:MET:HG3	2.05	0.56
1:A:233:ILE:CD1	1:A:233:ILE:H	2.19	0.56
1:A:887:THR:HA	1:A:953:MET:HG2	1.87	0.55
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.41	0.55
1:A:214:LYS:O	1:A:215:ILE:HD13	2.07	0.55
1:A:896:VAL:HG12	1:A:897:GLY:N	2.17	0.55
1:A:373:LEU:H	1:A:374:PRO:CD	2.20	0.54
1:A:226:ARG:O	1:A:227:SER:HB2	2.07	0.54
1:A:218:ASN:O	1:A:218:ASN:OD1	2.26	0.54
1:A:202:VAL:HG12	1:A:203:THR:N	2.21	0.54
1:A:1001:LYS:NZ	1:A:1001:LYS:HB3	2.23	0.54
1:A:233:ILE:N	1:A:233:ILE:HD12	2.20	0.54
1:A:180:LEU:C	1:A:183:PRO:HD2	2.27	0.54
1:A:271:VAL:HG23	1:A:282:VAL:HG12	1.90	0.54
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.37	0.54
1:A:373:LEU:N	1:A:374:PRO:CD	2.71	0.53
1:A:804:MET:HE3	1:A:810:PRO:CG	2.38	0.53
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.08	0.53
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.56	0.53
1:A:890:LYS:NZ	2:A:1:E52:C38	2.69	0.53
1:A:235:VAL:HG12	1:A:236:SER:N	2.23	0.53
1:A:750:LYS:HE3	1:A:809:LYS:N	2.23	0.53
1:A:807:LYS:HD2	1:A:807:LYS:H	1.72	0.53
1:A:825:ASN:N	1:A:825:ASN:ND2	2.55	0.53
1:A:756:LYS:O	1:A:758:ASP:OD2	2.27	0.53
1:A:988:THR:HB	1:A:989:PRO:HD2	1.91	0.53
1:A:850:ILE:O	1:A:854:ILE:HD13	2.09	0.53
1:A:371:PRO:HG2	1:A:511:GLU:O	2.08	0.53
1:A:622:LEU:HD21	1:A:651:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.57	0.52
1:A:176:THR:O	1:A:180:LEU:HG	2.10	0.52
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.77	0.52
1:A:1026:LEU:HD22	1:A:1026:LEU:O	2.08	0.52
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.09	0.52
1:A:229:THR:O	1:A:230:SER:HB3	2.09	0.52
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.42	0.52
1:A:174:GLU:HB3	1:A:178:ARG:HH12	1.75	0.52
1:A:1043:THR:N	1:A:1047:ASP:OD2	2.36	0.52
1:A:661:LEU:HD21	1:A:843:LEU:CD1	2.40	0.52
1:A:544:ARG:O	1:A:545:ALA:HB3	2.10	0.52
1:A:576:TRP:CD2	1:A:579:ARG:HD2	2.44	0.52
1:A:239:ASP:HB3	1:A:244:ILE:HG22	1.92	0.52
1:A:1055:LEU:O	1:A:1056:THR:C	2.49	0.52
1:A:549:ASN:HD22	1:A:550:GLN:NE2	2.08	0.52
1:A:544:ARG:CG	1:A:545:ALA:H	2.23	0.52
1:A:997:THR:CG2	1:A:998:SER:N	2.72	0.52
1:A:1043:THR:C	1:A:1045:LYS:N	2.64	0.51
1:A:890:LYS:CD	2:A:1:E52:C38	2.87	0.51
1:A:805:ALA:HB3	2:A:1:E52:C36	2.30	0.51
1:A:214:LYS:HZ2	1:A:300:GLY:HA2	1.72	0.51
1:A:690:ARG:HH11	1:A:690:ARG:HG3	1.74	0.51
1:A:161:ASP:O	1:A:164:ASP:HB3	2.10	0.51
1:A:1060:ASN:ND2	1:A:1062:GLU:HB2	2.22	0.51
1:A:804:MET:CE	1:A:831:ILE:HD12	2.40	0.51
1:A:583:LEU:O	1:A:583:LEU:HD23	2.11	0.51
1:A:1042:LEU:CD2	1:A:1048:ILE:HD11	2.40	0.51
1:A:685:GLY:O	1:A:688:ASN:O	2.28	0.51
1:A:657:LEU:HD21	1:A:691:ILE:HD12	1.92	0.50
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.42	0.50
1:A:208:PRO:HG2	1:A:211:LEU:HB2	1.92	0.50
1:A:379:LEU:HD13	1:A:380:THR:HG22	1.93	0.50
1:A:614:ARG:O	1:A:615:GLU:C	2.49	0.50
1:A:220:ILE:CD1	1:A:237:PRO:HG3	2.42	0.50
1:A:1009:PHE:CE2	1:A:1072:ILE:HD12	2.46	0.50
1:A:474:LEU:HA	1:A:525:HIS:N	2.27	0.50
1:A:202:VAL:CG1	1:A:203:THR:N	2.75	0.50
1:A:202:VAL:HG11	1:A:285:THR:HG21	1.94	0.50
1:A:293:VAL:O	1:A:297:LEU:HG	2.11	0.50
1:A:905:GLU:HG2	1:A:993:PHE:CZ	2.47	0.50
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:ALA:O	1:A:937:VAL:HG23	2.12	0.49
1:A:912:LYS:HA	1:A:921:PHE:CD1	2.46	0.49
1:A:757:TYR:HA	1:A:809:LYS:HZ1	1.77	0.49
1:A:576:TRP:CE2	1:A:579:ARG:HD2	2.47	0.49
1:A:831:ILE:HG12	1:A:881:ILE:HG12	1.94	0.49
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.42	0.49
1:A:923:ALA:O	1:A:926:GLU:HB3	2.12	0.49
1:A:235:VAL:HG12	1:A:236:SER:H	1.77	0.49
1:A:372:VAL:CG1	1:A:374:PRO:HD2	2.41	0.49
1:A:1002:THR:O	1:A:1003:SER:HB3	2.13	0.49
1:A:576:TRP:CZ2	1:A:579:ARG:HD2	2.48	0.49
1:A:498:ASN:C	1:A:498:ASN:OD1	2.50	0.49
1:A:767:LEU:HD12	1:A:803:VAL:HG23	1.95	0.49
1:A:229:THR:HG22	1:A:230:SER:H	1.76	0.49
1:A:544:ARG:HG2	1:A:545:ALA:N	2.27	0.49
1:A:246:GLN:C	1:A:248:PHE:H	2.14	0.49
1:A:896:VAL:HG21	1:A:903:LYS:HG3	1.94	0.49
1:A:544:ARG:CG	1:A:545:ALA:N	2.76	0.48
1:A:834:HIS:HA	1:A:875:LYS:O	2.13	0.48
1:A:691:ILE:HD12	1:A:691:ILE:N	2.28	0.48
1:A:1042:LEU:H	1:A:1042:LEU:HD12	1.79	0.48
1:A:150:PHE:HB2	1:A:319:ARG:NH1	2.28	0.48
1:A:397:ARG:NE	1:A:415:GLU:O	2.46	0.48
1:A:547:MET:HG2	1:A:578:PHE:CD2	2.48	0.48
1:A:466:LEU:CD1	1:A:476:ARG:HD3	2.43	0.48
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.95	0.48
1:A:470:ASP:OD2	1:A:474:LEU:HB2	2.13	0.48
1:A:804:MET:CE	1:A:810:PRO:HG2	2.44	0.48
1:A:555:LEU:O	1:A:559:ILE:HG12	2.14	0.48
1:A:896:VAL:HG22	1:A:903:LYS:HG3	1.96	0.48
1:A:912:LYS:O	1:A:912:LYS:HD2	2.13	0.48
1:A:927:ARG:HG3	1:A:927:ARG:HH11	1.78	0.48
1:A:1043:THR:HG22	1:A:1045:LYS:H	1.78	0.48
1:A:170:ASP:C	1:A:170:ASP:OD1	2.51	0.48
1:A:243:ALA:HA	1:A:246:GLN:HG3	1.95	0.48
1:A:833:LYS:HG3	1:A:834:HIS:N	2.29	0.48
1:A:890:LYS:CD	2:A:1:E52:O28	2.56	0.47
1:A:1032:SER:HB3	1:A:1048:ILE:HG23	1.96	0.47
1:A:757:TYR:HA	1:A:809:LYS:NZ	2.29	0.47
1:A:641:ARG:HE	1:A:670:GLU:CD	2.17	0.47
1:A:1026:LEU:HD22	1:A:1030:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LEU:HG	1:A:691:ILE:HD11	1.97	0.47
1:A:213:LYS:NZ	1:A:214:LYS:HB2	2.30	0.47
1:A:1032:SER:HB3	1:A:1048:ILE:CG2	2.45	0.47
1:A:373:LEU:H	1:A:374:PRO:HD2	1.76	0.47
1:A:233:ILE:HD11	1:A:248:PHE:CD1	2.50	0.47
1:A:184:ARG:CB	1:A:184:ARG:HH11	2.28	0.47
1:A:964:ASP:C	1:A:966:GLY:H	2.18	0.47
1:A:764:ILE:O	1:A:768:LYS:HG3	2.15	0.47
1:A:637:ASP:OD1	1:A:639:ASN:N	2.47	0.47
1:A:954:ILE:HG23	1:A:954:ILE:O	2.14	0.47
1:A:829:GLY:HA3	1:A:881:ILE:HD12	1.96	0.47
1:A:1060:ASN:ND2	1:A:1062:GLU:H	2.13	0.46
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.50	0.46
1:A:928:PHE:HE1	1:A:960:LEU:HD12	1.79	0.46
1:A:241:PRO:HG2	1:A:290:PHE:CZ	2.50	0.46
1:A:589:TYR:HD1	1:A:589:TYR:H	1.64	0.46
1:A:557:ALA:O	1:A:561:THR:HG23	2.15	0.46
1:A:1052:ARG:NH1	1:A:1052:ARG:HG2	2.31	0.46
1:A:1085:ASN:O	1:A:1087:PHE:N	2.49	0.46
1:A:661:LEU:HB2	1:A:698:PHE:CE1	2.50	0.46
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.50	0.46
1:A:685:GLY:HA2	1:A:691:ILE:HG22	1.98	0.46
1:A:741:MET:HE1	1:A:778:GLN:CB	2.39	0.46
1:A:1084:PHE:O	1:A:1087:PHE:CE1	2.69	0.45
1:A:779:LEU:O	1:A:780:PRO:C	2.54	0.45
1:A:862:LEU:HD11	1:A:1012:ILE:HG22	1.99	0.45
1:A:828:ILE:N	1:A:828:ILE:HD12	2.31	0.45
1:A:887:THR:O	1:A:891:ILE:HG12	2.17	0.45
1:A:389:HIS:O	1:A:392:GLN:HB3	2.16	0.45
1:A:239:ASP:O	1:A:287:ILE:HG12	2.17	0.45
1:A:927:ARG:HG3	1:A:927:ARG:NH1	2.31	0.45
1:A:699:LEU:O	1:A:703:ILE:HG13	2.17	0.45
1:A:174:GLU:OE1	1:A:178:ARG:NH1	2.50	0.45
1:A:614:ARG:HD2	1:A:618:ASP:OD1	2.17	0.45
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.99	0.45
1:A:1021:ARG:NE	1:A:1056:THR:CG2	2.80	0.45
1:A:925:VAL:O	1:A:929:VAL:HG23	2.17	0.45
1:A:1042:LEU:HD22	1:A:1042:LEU:C	2.37	0.44
1:A:276:GLY:HA3	1:A:822:ALA:HA	1.98	0.44
1:A:697:TRP:CH2	1:A:739:ILE:HD13	2.52	0.44
1:A:653:ASP:O	1:A:654:ASP:C	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:GLY:O	1:A:629:GLN:HG3	2.17	0.44
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.77	0.44
1:A:174:GLU:OE2	1:A:177:ARG:NH1	2.48	0.44
1:A:1035:LEU:CD1	1:A:1048:ILE:HD13	2.22	0.44
1:A:239:ASP:HB3	1:A:244:ILE:CG2	2.47	0.44
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.83	0.44
1:A:469:ILE:N	1:A:469:ILE:CD1	2.81	0.44
1:A:1054:ALA:C	1:A:1056:THR:H	2.21	0.44
1:A:838:LEU:HD12	1:A:838:LEU:HA	1.76	0.44
1:A:498:ASN:O	1:A:498:ASN:OD1	2.35	0.44
1:A:857:THR:O	1:A:858:GLU:HG2	2.18	0.44
1:A:480:TYR:HB2	1:A:518:ILE:HD11	1.98	0.44
1:A:815:PHE:O	1:A:827:THR:HB	2.18	0.44
1:A:219:CYS:HA	1:A:235:VAL:O	2.18	0.44
1:A:698:PHE:O	1:A:701:SER:HB3	2.18	0.44
1:A:804:MET:HE3	1:A:810:PRO:HG3	1.98	0.44
1:A:472:ARG:O	1:A:473:PHE:HB2	2.17	0.43
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.18	0.43
1:A:1056:THR:CG2	1:A:1056:THR:O	2.64	0.43
1:A:718:GLU:O	1:A:719:ALA:C	2.56	0.43
1:A:476:ARG:HB3	1:A:520:LEU:HD23	2.00	0.43
1:A:487:ILE:N	1:A:487:ILE:HD12	2.33	0.43
1:A:589:TYR:CD1	1:A:589:TYR:N	2.86	0.43
1:A:199:HIS:O	1:A:200:PRO:C	2.57	0.43
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.89	0.43
1:A:172:GLU:O	1:A:175:PHE:HB3	2.17	0.43
1:A:839:ARG:HA	1:A:842:MET:HE3	1.99	0.43
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.44	0.43
1:A:804:MET:CE	1:A:810:PRO:CG	2.96	0.43
1:A:807:LYS:H	1:A:807:LYS:CD	2.31	0.43
1:A:842:MET:HE2	1:A:871:SER:HB3	2.01	0.43
1:A:480:TYR:O	1:A:518:ILE:HD13	2.19	0.43
1:A:184:ARG:NH2	1:A:321:GLU:OE1	2.48	0.43
1:A:1086:TRP:O	1:A:1087:PHE:CD1	2.71	0.43
1:A:602:GLU:O	1:A:605:ALA:HB3	2.19	0.43
1:A:1017:TYR:CZ	1:A:1021:ARG:HD2	2.54	0.43
1:A:518:ILE:HD13	1:A:518:ILE:N	2.34	0.43
1:A:1042:LEU:CD1	1:A:1042:LEU:N	2.79	0.43
1:A:181:VAL:HG12	1:A:185:MET:CE	2.49	0.42
1:A:296:CYS:HB2	1:A:303:ILE:HD11	2.00	0.42
1:A:785:VAL:HG23	1:A:791:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:MET:N	1:A:1039:MET:SD	2.92	0.42
1:A:825:ASN:N	1:A:825:ASN:HD22	2.16	0.42
1:A:886:THR:HB	1:A:891:ILE:HD11	2.01	0.42
1:A:807:LYS:HD2	1:A:807:LYS:N	2.35	0.42
1:A:995:MET:O	1:A:1005:HIS:HB2	2.18	0.42
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.83	0.42
1:A:777:SER:O	1:A:778:GLN:HG2	2.18	0.42
1:A:1021:ARG:NE	1:A:1056:THR:HG22	2.28	0.42
1:A:753:SER:CB	1:A:809:LYS:HG3	2.50	0.42
1:A:707:ARG:HA	1:A:710:GLN:OE1	2.20	0.42
1:A:962:HIS:C	1:A:963:ILE:HG23	2.40	0.42
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.20	0.42
1:A:213:LYS:HD3	1:A:214:LYS:H	1.81	0.42
1:A:756:LYS:HB2	1:A:756:LYS:HE3	1.85	0.42
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.50	0.42
1:A:990:ASP:O	1:A:994:VAL:HG23	2.20	0.42
1:A:853:SER:O	1:A:856:GLU:HB3	2.19	0.41
1:A:614:ARG:HH11	1:A:646:GLN:NE2	2.17	0.41
1:A:184:ARG:CB	1:A:184:ARG:NH1	2.83	0.41
1:A:739:ILE:HG13	1:A:740:GLU:N	2.34	0.41
1:A:207:LEU:HD22	1:A:211:LEU:HB2	2.02	0.41
1:A:309:THR:HA	1:A:310:PRO:HD3	1.96	0.41
1:A:1043:THR:HG22	1:A:1045:LYS:N	2.36	0.41
1:A:774:LEU:C	1:A:776:ASN:N	2.73	0.41
1:A:181:VAL:O	1:A:184:ARG:HB3	2.20	0.41
1:A:862:LEU:HB3	1:A:934:GLY:HA3	2.03	0.41
1:A:552:ARG:O	1:A:556:GLU:HG3	2.21	0.41
1:A:463:TYR:HD2	1:A:487:ILE:CD1	2.31	0.41
1:A:583:LEU:C	1:A:583:LEU:HD23	2.41	0.41
1:A:610:LEU:HD23	1:A:610:LEU:HA	1.95	0.41
1:A:779:LEU:O	1:A:780:PRO:O	2.38	0.41
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.55	0.41
1:A:955:THR:HB	1:A:957:THR:HG22	2.03	0.41
1:A:808:LYS:HE3	1:A:836:ASP:OD1	2.21	0.41
1:A:787:TYR:HA	1:A:870:ILE:HD11	2.03	0.41
1:A:682:LEU:HD22	1:A:686:LEU:HD11	2.02	0.40
1:A:236:SER:O	1:A:239:ASP:N	2.48	0.40
1:A:690:ARG:NH1	1:A:690:ARG:HG3	2.36	0.40
1:A:600:GLN:CB	1:A:603:ILE:HD12	2.51	0.40
1:A:373:LEU:O	1:A:374:PRO:C	2.59	0.40
1:A:177:ARG:HG2	1:A:715:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:ILE:HG12	1:A:1051:ILE:HG23	2.04	0.40
1:A:914:LYS:HD2	1:A:956:GLU:OE2	2.21	0.40
1:A:391:GLN:HG3	1:A:502:LEU:HD21	2.02	0.40
1:A:921:PHE:O	1:A:925:VAL:HG23	2.22	0.40
1:A:547:MET:SD	1:A:552:ARG:HA	2.61	0.40
1:A:589:TYR:HB2	1:A:590:PRO:HD3	2.03	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	818/966 (85%)	715 (87%)	85 (10%)	18 (2%)	<b>8</b> 45

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	1086	TRP
1	A	227	SER
1	A	230	SER
1	A	758	ASP
1	A	1040	PRO
1	A	1044	SER
1	A	545	ALA
1	A	780	PRO
1	A	798	ILE
1	A	373	LEU
1	A	754	ALA
1	A	756	LYS
1	A	759	VAL
1	A	857	THR

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Mol	Chain	Res	Type
1	A	723	GLY
1	A	897	GLY
1	A	237	PRO

### 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	752/864 (87%)	702 (93%)	50 (7%)	21	61

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	MET
1	A	145	GLU
1	A	146	GLU
1	A	164	ASP
1	A	169	HIS
1	A	207	LEU
1	A	213	LYS
1	A	226	ARG
1	A	228	THR
1	A	229	THR
1	A	252	MET
1	A	269	ASP
1	A	298	LYS
1	A	322	GLU
1	A	373	LEU
1	A	375	ARG
1	A	379	LEU
1	A	476	ARG
1	A	477	ARG
1	A	498	ASN
1	A	518	ILE
1	A	521	ASP
1	A	570	GLU

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Mol	Chain	Res	Type
1	A	574	LEU
1	A	575	LEU
1	A	586	PRO
1	A	610	LEU
1	A	626	LEU
1	A	647	LYS
1	A	682	LEU
1	A	717	LEU
1	A	749	ILE
1	A	757	TYR
1	A	767	LEU
1	A	825	ASN
1	A	838	LEU
1	A	841	ASP
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	890	LYS
1	A	898	ASN
1	A	907	LEU
1	A	926	GLU
1	A	939	THR
1	A	967	HIS
1	A	1026	LEU
1	A	1042	LEU
1	A	1078	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	169	HIS
1	A	217	ASN
1	A	225	HIS
1	A	295	HIS
1	A	299	ASN
1	A	304	HIS
1	A	391	GLN
1	A	483	HIS
1	A	549	ASN
1	A	550	GLN

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Mol	Chain	Res	Type
1	A	634	ASN
1	A	646	GLN
1	A	743	GLN
1	A	766	GLN
1	A	769	GLN
1	A	773	ASN
1	A	825	ASN
1	A	840	GLN
1	A	962	HIS
1	A	967	HIS
1	A	1041	GLN
1	A	1060	ASN
1	A	1083	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	E52	A	1	-	25,52,52	5.86	10 (40%)	24,109,109	4.98	14 (58%)

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
2	E52	A	1	-	-	0/11/215/215	0/7/11/11

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	E52	O25-C14	-16.14	1.18	1.40
2	A	1	E52	C9-C8	-12.37	1.40	1.54
2	A	1	E52	F-C16	-12.09	1.21	1.36
2	A	1	E52	C11-C12	-10.07	1.41	1.52
2	A	1	E52	C6-C1	-8.31	1.42	1.52
2	A	1	E52	C11-C17	-7.37	1.41	1.51
2	A	1	E52	C9-C5	-5.98	1.42	1.54
2	A	1	E52	C6-C5	-3.83	1.48	1.53
2	A	1	E52	O24-C18	-2.23	1.18	1.23
2	A	1	E52	C3-C2	3.11	1.43	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	E52	C7-N22-C18	-5.26	117.90	123.36
2	A	1	E52	C5-C9-C8	-2.98	99.38	103.36
2	A	1	E52	C11-C12-C13	2.45	119.87	114.77
2	A	1	E52	O23-C1-C6	2.92	117.88	111.02
2	A	1	E52	C37-C35-N39	3.02	115.91	108.26
2	A	1	E52	C15-N20-C10	5.07	117.81	113.26
2	A	1	E52	C9-C5-C4	5.58	111.81	102.87
2	A	1	E52	C8-C10-N20	6.48	118.57	109.26
2	A	1	E52	C9-C8-N21	6.83	115.90	103.50
2	A	1	E52	O23-C1-C2	7.13	121.57	109.94
2	A	1	E52	C6-C1-C2	8.17	120.53	111.34
2	A	1	E52	C9-C8-C10	8.75	126.04	113.38
2	A	1	E52	C16-C15-N20	9.55	120.30	110.19
2	A	1	E52	C10-C8-N21	9.75	117.91	108.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	E52	20	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	836/966 (86%)	0.32	56 (6%) 21 12	46, 98, 156, 194	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	899	THR	11.8
1	A	898	ASN	11.4
1	A	528	ALA	7.9
1	A	143	MET	7.6
1	A	1044	SER	6.4
1	A	374	PRO	5.0
1	A	763	VAL	4.9
1	A	1086	TRP	4.7
1	A	376	ASN	4.4
1	A	1041	GLN	4.4
1	A	755	GLU	4.4
1	A	373	LEU	4.2
1	A	228	THR	4.2
1	A	378	ASP	4.0
1	A	270	PHE	3.8
1	A	757	TYR	3.7
1	A	404	PHE	3.6
1	A	322	GLU	3.6
1	A	252	MET	3.5
1	A	527	ILE	3.5
1	A	526	PRO	3.5
1	A	307	LEU	3.4
1	A	1082	VAL	3.4
1	A	545	ALA	3.4
1	A	377	THR	3.3
1	A	211	LEU	3.3
1	A	320	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	489	GLY	3.2
1	A	816	LYS	3.2
1	A	214	LYS	2.9
1	A	894	SER	2.9
1	A	544	ARG	2.8
1	A	267	GLU	2.8
1	A	859	SER	2.8
1	A	375	ARG	2.7
1	A	825	ASN	2.7
1	A	764	ILE	2.6
1	A	767	LEU	2.6
1	A	213	LYS	2.6
1	A	232	THR	2.5
1	A	948	HIS	2.5
1	A	916	PRO	2.5
1	A	215	ILE	2.4
1	A	998	SER	2.4
1	A	248	PHE	2.3
1	A	220	ILE	2.3
1	A	358	ASP	2.2
1	A	237	PRO	2.2
1	A	1046	GLU	2.2
1	A	144	SER	2.1
1	A	216	ALA	2.1
1	A	766	GLN	2.1
1	A	253	ALA	2.1
1	A	233	ILE	2.1
1	A	795	ALA	2.0
1	A	900	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	E52	A	1	42/42	0.93	0.21	-1.22	94,104,119,119	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.