



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:48 AM GMT

PDB ID : 2O9I
Title : Crystal Structure of the Human Pregnane X Receptor LBD in complex with an SRC-1 coactivator peptide and T0901317
Authors : Xue, Y.; Redinbo, M.R.
Deposited on : 2006-12-13
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 ⓘ 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) : 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

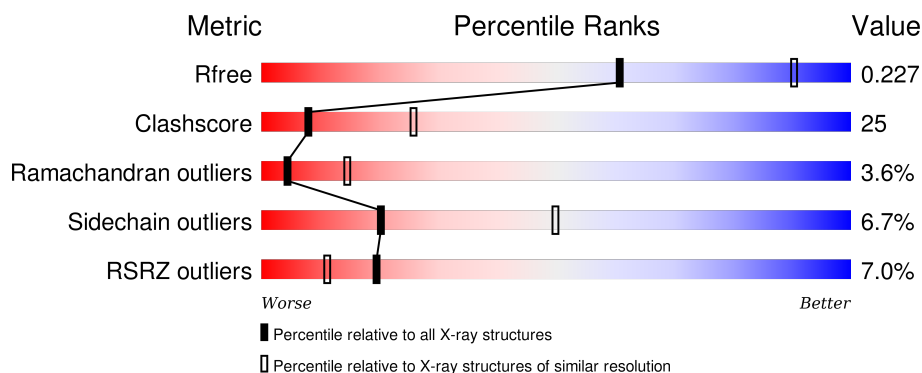
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 $\leq 5\%$. 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	293	<div> <div>5%</div> <div>54% 35% 6% 5%</div> </div>
1	B	293	<div> <div>6%</div> <div>51% 38% 6% 5%</div> </div>
2	C	15	<div> <div>40%</div> <div>20% 60% 20%</div> </div>
2	D	15	<div> <div>7%</div> <div>47% 40% 13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	444	A	2	-	-	-	X
3	444	B	1	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4990 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 Orphan nuclear receptor PXR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2265	1455	386	407	17			
1	B	279	Total	C	N	O	S	0	0	0
			2265	1455	386	407	17			

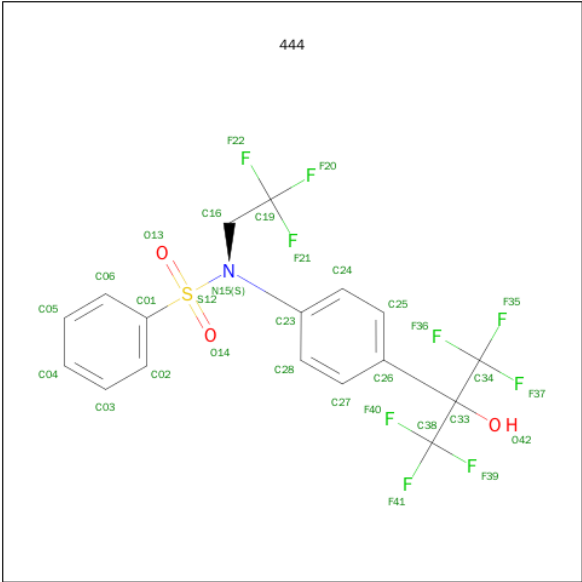
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	SER	CYS	ENGINEERED	UNP O75469
B	1284	SER	CYS	ENGINEERED	UNP O75469

- Molecule 2 is a protein called Nuclear Receptor Coactivator 1 isoform 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	0	0	0
			131	82	27	22			
2	D	15	Total	C	N	O	0	0	0
			132	82	27	23			

- Molecule 3 is N-(2,2,2-TRIFLUOROETHYL)-N-{4-[2,2,2-TRIFLUORO-1-HYDROXY-1-(TRIFLUOROMETHYL)ETHYL]PHENYL}BENZENESULFONAMIDE (three-letter code: 444) (formula: C₁₇H₁₂F₉NO₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	S	0	0
			31	17	9	1	3	1		
3	A	1	Total	C	F	N	O	S	0	0
			31	17	9	1	3	1		

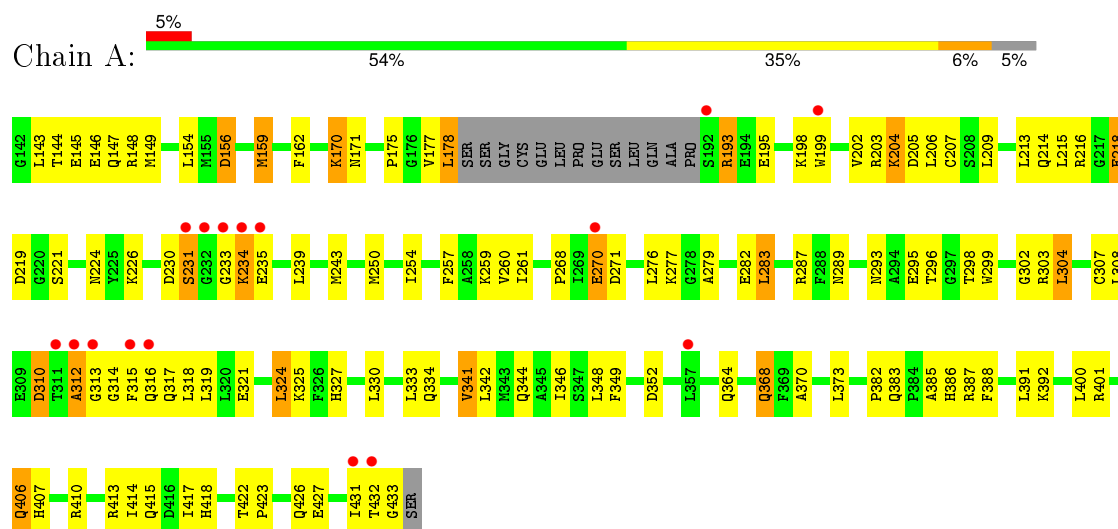
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	66	Total	O	0	0
			66	66		
4	C	1	Total	O	0	0
			1	1		
4	D	6	Total	O	0	0
			6	6		

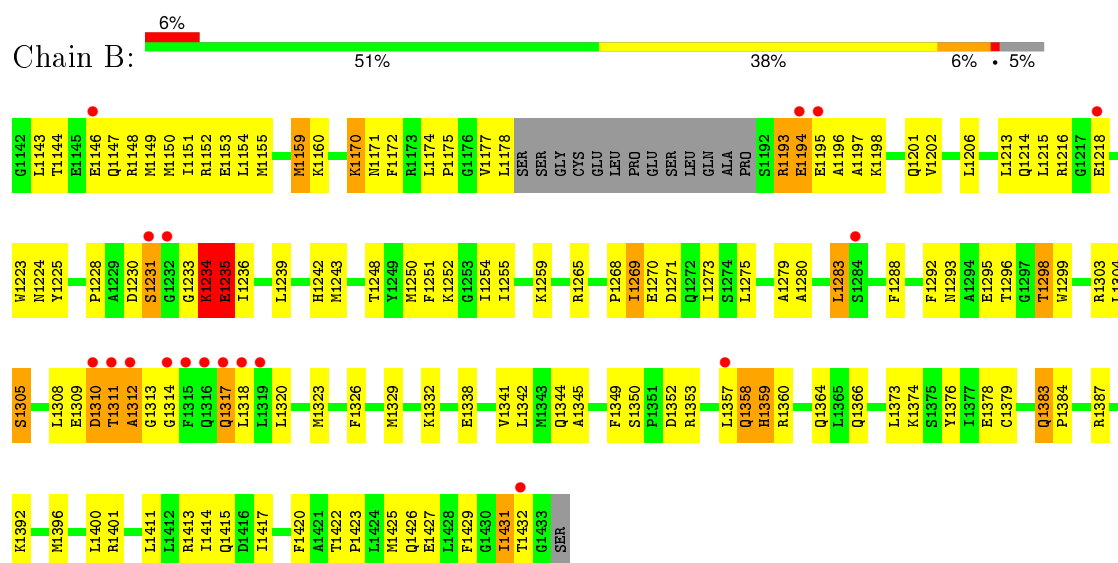
3 Residue-property plots

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: Orphan nuclear receptor PXR

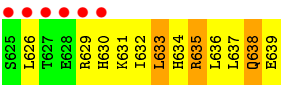


• Molecule 1: Orphan nuclear receptor PXR



• Molecule 2: Nuclear Receptor Coactivator 1 isoform 3





● Molecule 2: Nuclear Receptor Coactivator 1 isoform 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.98Å 90.62Å 105.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 37.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.80) 98.4 (37.31-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.96 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.240 0.225 , 0.227	Depositor DCC
R_{free} test set	1029 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 20118 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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:
444

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	0.47	1/2315 (0.0%)	0.61	0/3117
1	B	0.43	0/2315	0.57	0/3117
2	C	0.43	0/132	0.57	0/175
2	D	0.26	0/133	0.44	0/175
All	All	0.44	1/4895 (0.0%)	0.58	0/6584

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	GLU	CD-OE1	-5.65	1.19	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2265	0	2273	111	1
1	B	2265	0	2273	126	0
2	C	131	0	139	13	0
2	D	132	0	139	11	0
3	A	31	0	12	3	0
3	B	31	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	62	0	0	8	0
4	B	66	0	0	3	0
4	C	1	0	0	0	0
4	D	6	0	0	0	0
All	All	4990	0	4848	241	1

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 25.

All (241) 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:202:VAL:HG21	1:A:417:ILE:HD12	1.43	0.95
1:B:1360:ARG:HH21	1:B:1364:GLN:HG2	1.35	0.87
1:B:1144:THR:OG1	1:B:1146:GLU:HG2	1.75	0.85
1:B:1317:GLN:HE22	1:B:1318:LEU:HD23	1.42	0.84
1:B:1195:GLU:HG3	1:B:1198:LYS:HD2	1.64	0.80
1:A:193:ARG:CZ	1:A:193:ARG:HA	2.12	0.80
1:B:1254:ILE:HD12	1:B:1283:LEU:HB3	1.65	0.78
1:B:1383:GLN:H	1:B:1383:GLN:CD	1.86	0.78
1:B:1296:THR:OG1	1:B:1298:THR:HG23	1.84	0.77
1:B:1202:VAL:HG21	1:B:1417:ILE:HD12	1.67	0.77
1:A:219:ASP:HB2	1:B:1235:GLU:HG3	1.68	0.75
1:B:1214:GLN:HE21	1:B:1216:ARG:HH11	1.33	0.73
1:A:202:VAL:CG2	1:A:417:ILE:HD12	2.18	0.73
1:B:1360:ARG:HH21	1:B:1364:GLN:CG	2.03	0.71
1:A:296:THR:O	1:A:298:THR:HG23	1.90	0.71
1:A:144:THR:OG1	1:A:146:GLU:HG2	1.91	0.71
1:A:387:ARG:O	1:A:388:PHE:HB2	1.88	0.71
1:B:1431:ILE:HD12	1:B:1431:ILE:H	1.56	0.71
1:A:144:THR:OG1	1:A:147:GLN:HG3	1.91	0.70
2:D:1626:LEU:HA	2:D:1629:ARG:NH1	2.06	0.69
1:A:282:GLU:HG2	1:A:400:LEU:HG	1.75	0.69
1:B:1216:ARG:O	1:B:1303:ARG:HD2	1.93	0.68
1:A:427:GLU:OE2	2:C:633:LEU:HB2	1.95	0.66
1:A:259:LYS:HD3	2:C:637:LEU:O	1.97	0.65
1:A:148:ARG:HD3	4:A:3106:HOH:O	1.97	0.65
1:A:178:LEU:H	1:A:178:LEU:HD22	1.62	0.65
1:A:298:THR:HG22	1:A:307:CYS:HA	1.77	0.65
1:B:1374:LYS:O	1:B:1378:GLU:HG3	1.97	0.65
1:A:279:ALA:O	1:A:283:LEU:HD23	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLU:HG2	1:B:1178:LEU:O	1.99	0.63
1:A:283:LEU:CD1	1:A:344:GLN:HB3	2.29	0.62
1:B:1312:ALA:O	1:B:1314:GLY:N	2.32	0.62
4:A:3032:HOH:O	1:B:1178:LEU:HD21	1.99	0.62
1:B:1422:THR:O	1:B:1426:GLN:HG3	2.00	0.62
1:A:204:LYS:HA	1:A:204:LYS:NZ	2.16	0.61
1:B:1431:ILE:HG22	1:B:1431:ILE:O	2.01	0.61
1:B:1213:LEU:HD23	1:B:1214:GLN:N	2.16	0.60
1:A:364:GLN:HE21	1:A:368:GLN:HE22	1.50	0.60
1:A:199:TRP:O	1:A:203:ARG:HG3	2.02	0.60
1:A:277:LYS:HD3	2:C:630:HIS:NE2	2.17	0.59
1:A:383:GLN:CD	1:A:383:GLN:H	2.05	0.59
1:B:1201:GLN:HG3	1:B:1413:ARG:HH11	1.67	0.59
1:A:283:LEU:HD13	1:A:344:GLN:HB3	1.85	0.58
1:B:1149:MET:HE3	1:B:1152:ARG:HB2	1.86	0.58
1:B:1415:GLN:HG2	1:B:1431:ILE:HG12	1.84	0.57
1:A:214:GLN:HG3	1:A:224:ASN:HD22	1.70	0.57
2:D:1626:LEU:HA	2:D:1629:ARG:HH11	1.70	0.57
1:B:1269:ILE:O	1:B:1273:ILE:HG13	2.06	0.56
1:B:1273:ILE:HG23	2:D:1633:LEU:HD13	1.88	0.56
1:B:1170:LYS:HB2	4:B:3056:HOH:O	2.06	0.56
1:A:170:LYS:HB3	1:A:170:LYS:NZ	2.21	0.56
1:B:1193:ARG:O	1:B:1196:ALA:N	2.39	0.56
1:B:1218:GLU:HG2	1:B:1303:ARG:NH2	2.21	0.56
1:B:1144:THR:HG1	1:B:1146:GLU:HG2	1.71	0.56
1:A:422:THR:O	1:A:426:GLN:HG3	2.07	0.55
1:B:1255:ILE:HG22	1:B:1259:LYS:NZ	2.22	0.55
1:A:193:ARG:HA	1:A:193:ARG:NE	2.20	0.55
1:A:145:GLU:HG3	1:A:149:MET:HE2	1.89	0.55
1:A:313:GLY:HA3	1:A:317:GLN:HB2	1.89	0.55
1:A:216:ARG:NH2	1:A:302:GLY:O	2.40	0.55
1:A:143:LEU:HB3	1:A:147:GLN:HB2	1.88	0.55
1:B:1317:GLN:O	1:B:1320:LEU:HB2	2.07	0.54
1:B:1265:ARG:HB3	1:B:1265:ARG:HH11	1.72	0.54
1:B:1242:HIS:HD2	1:B:1243:MET:CE	2.20	0.54
1:A:175:PRO:HD2	1:B:1223:TRP:HZ2	1.73	0.54
1:B:1283:LEU:CD1	1:B:1344:GLN:HB3	2.37	0.54
1:A:144:THR:HG1	1:A:147:GLN:HG3	1.72	0.54
1:A:388:PHE:O	1:A:392:LYS:HG3	2.07	0.54
1:B:1159:MET:HE2	1:B:1160:LYS:HA	1.90	0.54
1:B:1159:MET:HG3	1:B:1160:LYS:N	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:THR:HG22	1:A:307:CYS:SG	2.49	0.53
1:A:239:LEU:O	1:A:243:MET:HG2	2.09	0.53
1:B:1214:GLN:NE2	1:B:1216:ARG:HH11	2.05	0.52
1:A:204:LYS:HA	1:A:204:LYS:HZ1	1.72	0.52
1:B:1384:PRO:O	1:B:1387:ARG:HG3	2.09	0.52
1:B:1268:PRO:O	1:B:1270:GLU:N	2.43	0.51
1:B:1175:PRO:HG3	1:B:1239:LEU:HD13	1.91	0.51
1:B:1342:LEU:HD13	1:B:1373:LEU:HA	1.92	0.51
1:A:213:LEU:HD23	1:A:214:GLN:N	2.25	0.51
1:A:233:GLY:O	1:A:235:GLU:N	2.43	0.51
1:B:1215:LEU:CD2	1:B:1304:LEU:HG	2.40	0.51
1:A:215:LEU:HD13	1:B:1177:VAL:HG23	1.93	0.51
1:A:415:GLN:HG2	1:A:431:ILE:HD13	1.91	0.51
1:B:1144:THR:OG1	1:B:1147:GLN:HG3	2.10	0.51
1:A:407:HIS:NE2	3:A:2:444:H27	2.26	0.51
1:B:1317:GLN:HA	1:B:1320:LEU:HD12	1.94	0.50
1:A:277:LYS:HD3	2:C:630:HIS:CD2	2.46	0.50
1:A:382:PRO:HD2	1:A:383:GLN:HE22	1.75	0.50
1:B:1206:LEU:HD21	1:B:1414:ILE:HD13	1.93	0.50
1:B:1146:GLU:CG	1:B:1147:GLN:N	2.75	0.50
1:B:1213:LEU:HD21	1:B:1215:LEU:HD21	1.94	0.49
1:A:312:ALA:O	1:A:317:GLN:HG2	2.11	0.49
1:B:1292:PHE:HB2	1:B:1299:TRP:CD1	2.47	0.49
1:A:230:ASP:O	1:A:231:SER:HB3	2.10	0.49
1:A:342:LEU:HD13	1:A:373:LEU:HA	1.93	0.49
1:A:304:LEU:HD23	1:A:304:LEU:H	1.77	0.49
1:B:1230:ASP:O	1:B:1231:SER:HB3	2.12	0.49
1:B:1350:SER:O	1:B:1353:ARG:HG2	2.12	0.49
1:B:1230:ASP:O	1:B:1231:SER:CB	2.60	0.49
1:B:1193:ARG:O	1:B:1195:GLU:N	2.45	0.49
1:B:1202:VAL:CG2	1:B:1417:ILE:HD12	2.40	0.49
1:B:1353:ARG:NH1	1:B:1401:ARG:NH1	2.61	0.49
1:B:1338:GLU:O	1:B:1341:VAL:HG12	2.12	0.49
1:B:1242:HIS:HD2	1:B:1243:MET:HE2	1.77	0.49
1:B:1201:GLN:CG	1:B:1413:ARG:HH11	2.26	0.48
1:B:1175:PRO:HG2	1:B:1225:TYR:CE2	2.48	0.48
1:B:1153:GLU:HG2	4:B:3043:HOH:O	2.12	0.48
1:A:383:GLN:O	1:A:385:ALA:N	2.46	0.48
1:A:214:GLN:HG3	1:A:224:ASN:ND2	2.27	0.48
1:A:383:GLN:C	1:A:385:ALA:N	2.67	0.48
1:B:1177:VAL:HG13	1:B:1177:VAL:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASN:OD1	1:A:295:GLU:HB3	2.13	0.48
1:B:1314:GLY:O	1:B:1317:GLN:HB3	2.14	0.48
2:C:634:HIS:NE2	2:C:638:GLN:OE1	2.47	0.48
1:B:1193:ARG:NH2	1:B:1197:ALA:H	2.10	0.48
1:A:289:ASN:ND2	1:A:330:LEU:HG	2.29	0.48
1:B:1151:ILE:O	1:B:1155:MET:HB2	2.14	0.48
1:B:1273:ILE:HD12	2:D:1627:THR:HG22	1.96	0.48
1:B:1349:PHE:O	1:B:1366:GLN:HB2	2.14	0.48
1:B:1149:MET:CE	1:B:1152:ARG:HD2	2.44	0.47
1:B:1248:THR:HG22	1:B:1252:LYS:HE3	1.96	0.47
1:B:1218:GLU:HA	1:B:1303:ARG:NH2	2.30	0.47
1:A:145:GLU:O	1:A:149:MET:HE2	2.15	0.47
1:A:178:LEU:HD13	4:A:3042:HOH:O	2.13	0.47
1:A:175:PRO:HD2	1:B:1223:TRP:CZ2	2.50	0.47
1:B:1357:LEU:C	1:B:1359:HIS:H	2.17	0.47
1:B:1159:MET:HE2	1:B:1160:LYS:CA	2.45	0.47
1:B:1155:MET:HE3	1:B:1155:MET:HA	1.97	0.47
1:A:250:MET:O	1:A:254:ILE:HG12	2.15	0.46
1:A:215:LEU:HD13	1:B:1177:VAL:CG2	2.45	0.46
1:B:1271:ASP:O	1:B:1275:LEU:HG	2.16	0.46
2:C:637:LEU:C	2:C:638:GLN:HE21	2.18	0.46
1:B:1265:ARG:CB	1:B:1265:ARG:NH1	2.78	0.46
1:A:254:ILE:O	1:A:257:PHE:HB3	2.14	0.46
1:A:193:ARG:NH2	1:A:193:ARG:HB2	2.30	0.46
1:A:407:HIS:HE2	3:A:2:444:H27	1.79	0.46
1:B:1392:LYS:O	1:B:1396:MET:HG2	2.15	0.46
1:B:1317:GLN:NE2	1:B:1318:LEU:HA	2.30	0.46
1:B:1283:LEU:HD11	1:B:1344:GLN:HB3	1.98	0.46
1:A:195:GLU:O	1:A:198:LYS:HB2	2.16	0.46
1:A:307:CYS:HB3	4:A:3107:HOH:O	2.17	0.45
2:D:1626:LEU:HD12	2:D:1629:ARG:NH1	2.31	0.45
1:A:193:ARG:NH1	4:A:3073:HOH:O	2.50	0.45
1:A:391:LEU:HG	4:A:3039:HOH:O	2.17	0.45
1:B:1283:LEU:HD13	1:B:1344:GLN:HB3	1.99	0.45
1:B:1149:MET:HE3	1:B:1152:ARG:HD2	1.98	0.45
1:B:1216:ARG:HH12	1:B:1305:SER:HB2	1.82	0.45
1:B:1148:ARG:O	1:B:1152:ARG:HG3	2.17	0.45
1:B:1270:GLU:OE2	2:D:1627:THR:HG21	2.17	0.45
1:B:1251:PHE:O	1:B:1255:ILE:HG13	2.17	0.45
1:A:346:ILE:HD11	1:A:370:ALA:HA	1.99	0.45
1:B:1193:ARG:HD3	1:B:1194:GLU:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASP:O	1:A:410:ARG:NH1	2.49	0.45
1:A:156:ASP:O	1:A:159:MET:HG3	2.18	0.45
1:B:1329:MET:O	1:B:1332:LYS:HB3	2.17	0.45
1:A:259:LYS:HZ1	2:C:639:GLU:HG3	1.82	0.44
1:A:231:SER:HA	4:A:3113:HOH:O	2.17	0.44
1:A:206:LEU:HD21	1:A:414:ILE:HD13	1.99	0.44
1:A:215:LEU:HD23	1:A:304:LEU:HB3	1.99	0.44
1:A:235:GLU:H	1:A:235:GLU:CD	2.20	0.44
1:A:209:LEU:HD11	1:A:410:ARG:NH1	2.31	0.44
1:A:234:LYS:HE3	1:A:418:HIS:HD2	1.83	0.44
1:A:382:PRO:HG2	1:A:383:GLN:NE2	2.32	0.44
1:A:145:GLU:OE2	1:A:148:ARG:NH2	2.51	0.44
1:A:209:LEU:HD22	3:A:2:444:F21	2.08	0.44
1:B:1193:ARG:O	1:B:1194:GLU:C	2.56	0.44
1:B:1177:VAL:HG22	1:B:1178:LEU:HG	2.00	0.44
1:B:1170:LYS:O	1:B:1171:ASN:HB2	2.17	0.44
1:A:268:PRO:O	1:A:271:ASP:N	2.51	0.44
1:A:299:TRP:HZ2	1:A:327:HIS:CD2	2.35	0.44
1:B:1293:ASN:OD1	1:B:1295:GLU:HB2	2.18	0.44
2:D:1629:ARG:HD3	2:D:1629:ARG:H	1.83	0.44
1:B:1265:ARG:CB	1:B:1265:ARG:HH11	2.30	0.44
1:A:431:ILE:O	1:A:433:GLY:N	2.50	0.44
1:B:1193:ARG:HH21	1:B:1197:ALA:N	2.14	0.44
1:B:1149:MET:HE3	1:B:1149:MET:HA	2.00	0.44
1:A:303:ARG:HH11	1:A:303:ARG:HG2	1.82	0.44
1:A:143:LEU:HD12	1:A:143:LEU:N	2.33	0.43
2:C:626:LEU:O	2:C:630:HIS:ND1	2.51	0.43
1:B:1239:LEU:O	1:B:1243:MET:HG2	2.18	0.43
2:D:1635:ARG:O	2:D:1639:GLU:HG2	2.18	0.43
1:B:1175:PRO:CG	1:B:1239:LEU:HD13	2.48	0.43
1:A:170:LYS:O	1:A:171:ASN:HB2	2.17	0.43
1:A:298:THR:CG2	1:A:307:CYS:SG	3.06	0.43
1:A:333:LEU:O	1:A:334:GLN:C	2.57	0.43
1:A:383:GLN:C	1:A:385:ALA:H	2.21	0.43
1:B:1213:LEU:C	1:B:1213:LEU:HD23	2.39	0.43
1:B:1255:ILE:HG22	1:B:1259:LYS:HZ2	1.83	0.43
1:B:1309:GLU:O	1:B:1310:ASP:C	2.57	0.43
1:B:1172:PHE:HE1	1:B:1174:LEU:HD21	1.84	0.43
2:C:629:ARG:HH11	2:C:629:ARG:HB3	1.84	0.42
1:B:1326:PHE:CE2	1:B:1400:LEU:HD13	2.54	0.42
1:B:1427:GLU:OE1	2:D:1630:HIS:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PRO:O	1:A:426:GLN:HB2	2.18	0.42
1:B:1425:MET:O	1:B:1429:PHE:HD1	2.02	0.42
1:A:310:ASP:HB3	4:A:3100:HOH:O	2.20	0.42
1:A:315:PHE:CZ	1:A:319:LEU:HD11	2.54	0.42
2:C:632:ILE:O	2:C:636:LEU:N	2.49	0.42
1:B:1193:ARG:HH21	1:B:1197:ALA:H	1.68	0.42
1:A:312:ALA:C	1:A:314:GLY:H	2.22	0.42
1:A:257:PHE:O	1:A:261:ILE:HG13	2.20	0.42
1:A:423:PRO:HA	1:A:426:GLN:NE2	2.34	0.42
1:B:1250:MET:HG3	1:B:1288:PHE:CE1	2.55	0.42
1:B:1312:ALA:C	1:B:1314:GLY:H	2.23	0.42
1:A:234:LYS:HE3	1:A:418:HIS:CD2	2.55	0.42
1:B:1309:GLU:O	1:B:1311:THR:N	2.53	0.42
1:A:321:GLU:HG3	1:A:324:LEU:H	1.85	0.42
1:A:276:LEU:HA	1:A:276:LEU:HD23	1.80	0.42
1:A:254:ILE:HD11	1:A:287:ARG:HD2	2.02	0.42
1:A:387:ARG:O	1:A:388:PHE:CB	2.61	0.41
1:B:1423:PRO:HB2	2:D:1632:ILE:CD1	2.50	0.41
1:A:348:LEU:HD23	1:A:349:PHE:CE1	2.55	0.41
1:B:1279:ALA:O	1:B:1280:ALA:C	2.57	0.41
1:B:1358:GLN:C	1:B:1360:ARG:H	2.23	0.41
1:B:1231:SER:C	1:B:1233:GLY:H	2.22	0.41
1:B:1411:LEU:HD12	1:B:1420:PHE:HZ	1.85	0.41
1:A:234:LYS:CE	1:A:418:HIS:HD2	2.34	0.41
1:B:1376:TYR:CD1	1:B:1376:TYR:C	2.93	0.41
1:B:1234:LYS:C	1:B:1236:ILE:H	2.23	0.41
1:B:1150:MET:O	1:B:1154:LEU:HD13	2.21	0.41
1:B:1202:VAL:HG23	4:B:3044:HOH:O	2.21	0.41
1:B:1177:VAL:O	1:B:1178:LEU:HB2	2.21	0.41
1:A:221:SER:HB2	1:B:1225:TYR:CE1	2.56	0.41
1:B:1342:LEU:O	1:B:1345:ALA:HB3	2.21	0.41
1:A:406:GLN:HE22	1:A:413:ARG:HH22	1.69	0.41
2:C:635:ARG:C	2:C:635:ARG:HD3	2.41	0.41
1:B:1143:LEU:HD13	1:B:1379:CYS:SG	2.61	0.41
1:B:1358:GLN:O	1:B:1360:ARG:N	2.54	0.41
1:A:383:GLN:O	1:A:386:HIS:N	2.45	0.40
1:A:319:LEU:HD22	1:A:325:LYS:HG3	2.04	0.40
1:A:318:LEU:O	1:A:321:GLU:HB3	2.21	0.40
1:A:352:ASP:OD2	1:A:401:ARG:CZ	2.70	0.40
1:A:177:VAL:HG11	1:B:1215:LEU:HD13	2.02	0.40
1:A:170:LYS:HB3	1:A:170:LYS:HZ3	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD23	1:A:341:VAL:HG13	2.02	0.40
1:A:226:LYS:HE3	1:A:226:LYS:HB2	1.69	0.40
1:B:1146:GLU:HG2	1:B:1147:GLN:HG3	2.02	0.40
1:B:1243:MET:SD	3:B:1:444:H05	2.62	0.40
1:A:276:LEU:HD13	2:C:633:LEU:HD21	2.03	0.40
2:C:629:ARG:C	2:C:630:HIS:ND1	2.75	0.40
1:B:1427:GLU:OE2	2:D:1632:ILE:HB	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:OE1	1:A:316:GLN:OE1[3_545]	1.66	0.54

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	275/293 (94%)	245 (89%)	25 (9%)	5 (2%)	11	34
1	B	275/293 (94%)	244 (89%)	16 (6%)	15 (6%)	2	6
2	C	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1	2
2	D	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
All	All	576/616 (94%)	510 (88%)	45 (8%)	21 (4%)	4	14

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	LYS
1	A	432	THR
1	B	1194	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1231	SER
1	B	1310	ASP
1	B	1312	ALA
1	B	1313	GLY
1	A	207	CYS
1	B	1234	LYS
1	B	1269	ILE
1	B	1311	THR
1	B	1431	ILE
1	B	1358	GLN
2	C	631	LYS
1	A	231	SER
1	B	1228	PRO
1	B	1235	GLU
1	B	1352	ASP
1	B	1359	HIS
1	A	312	ALA
1	B	1383	GLN

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	248/260 (95%)	231 (93%)	17 (7%)	19	48
1	B	248/260 (95%)	235 (95%)	13 (5%)	29	62
2	C	15/15 (100%)	12 (80%)	3 (20%)	1	5
2	D	15/15 (100%)	13 (87%)	2 (13%)	5	14
All	All	526/550 (96%)	491 (93%)	35 (7%)	20	50

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	ASP
1	A	159	MET
1	A	162	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	170	LYS
1	A	178	LEU
1	A	193	ARG
1	A	204	LYS
1	A	218	GLU
1	A	260	VAL
1	A	283	LEU
1	A	304	LEU
1	A	308	LEU
1	A	310	ASP
1	A	324	LEU
1	A	341	VAL
1	A	368	GLN
1	A	406	GLN
1	B	1159	MET
1	B	1170	LYS
1	B	1193	ARG
1	B	1224	ASN
1	B	1234	LYS
1	B	1235	GLU
1	B	1283	LEU
1	B	1298	THR
1	B	1305	SER
1	B	1308	LEU
1	B	1317	GLN
1	B	1323	MET
1	B	1432	THR
2	C	633	LEU
2	C	635	ARG
2	C	638	GLN
2	D	1629	ARG
2	D	1633	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	201	GLN
1	A	224	ASN
1	A	289	ASN
1	A	364	GLN
1	A	383	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	418	HIS
1	A	426	GLN
1	B	1171	ASN
1	B	1214	GLN
1	B	1224	ASN
1	B	1289	ASN
1	B	1317	GLN
1	B	1426	GLN
2	C	638	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	444	A	2	-	32,32,32	5.93	21 (65%)	51,52,52	2.74	11 (21%)
3	444	B	1	-	32,32,32	6.05	20 (62%)	51,52,52	2.80	12 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	444	A	2	-	-	0/44/45/45	0/2/2/2
3	444	B	1	-	-	0/44/45/45	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	444	S12-N15	-2.62	1.61	1.64
3	A	2	444	C25-C24	2.27	1.42	1.38
3	A	2	444	C16-C19	2.44	1.53	1.50
3	A	2	444	C38-C33	2.55	1.59	1.54
3	B	1	444	C01-S12	2.70	1.80	1.76
3	A	2	444	C27-C28	2.81	1.43	1.38
3	B	1	444	C27-C28	2.83	1.43	1.38
3	B	1	444	C38-C33	3.10	1.60	1.54
3	B	1	444	C25-C24	3.33	1.44	1.38
3	A	2	444	C16-N15	3.40	1.54	1.48
3	A	2	444	C01-S12	3.49	1.81	1.76
3	B	1	444	C16-C19	3.61	1.55	1.50
3	B	1	444	C16-N15	3.94	1.55	1.48
3	B	1	444	C05-C06	4.17	1.47	1.38
3	A	2	444	C05-C06	4.24	1.47	1.38
3	A	2	444	C05-C04	4.41	1.49	1.38
3	A	2	444	C28-C23	4.48	1.48	1.39
3	B	1	444	C05-C04	4.51	1.49	1.38
3	B	1	444	C04-C03	4.52	1.49	1.38
3	B	1	444	C28-C23	4.57	1.48	1.39
3	A	2	444	C04-C03	4.68	1.50	1.38
3	B	1	444	C03-C02	5.12	1.49	1.38
3	A	2	444	C03-C02	5.15	1.49	1.38
3	B	1	444	C06-C01	6.66	1.49	1.38
3	A	2	444	C06-C01	6.84	1.50	1.38
3	A	2	444	C33-C26	7.53	1.65	1.53
3	A	2	444	C24-C23	7.58	1.54	1.39
3	B	1	444	C24-C23	7.79	1.54	1.39
3	B	1	444	C02-C01	7.91	1.51	1.38
3	A	2	444	C02-C01	7.92	1.51	1.38
3	A	2	444	C25-C26	7.96	1.51	1.39
3	A	2	444	C27-C26	8.17	1.52	1.39
3	B	1	444	C33-C26	8.29	1.66	1.53
3	B	1	444	C25-C26	8.32	1.52	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	444	C27-C26	8.53	1.52	1.39
3	B	1	444	O14-S12	12.90	1.59	1.43
3	A	2	444	O14-S12	12.98	1.60	1.43
3	B	1	444	O13-S12	13.52	1.60	1.43
3	A	2	444	O13-S12	13.55	1.60	1.43
3	A	2	444	C23-N15	15.72	1.64	1.44
3	B	1	444	C23-N15	16.23	1.64	1.44

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	444	O14-S12-O13	-8.87	104.17	119.47
3	B	1	444	O14-S12-O13	-8.65	104.55	119.47
3	B	1	444	O14-S12-C01	-7.61	98.13	108.00
3	A	2	444	C16-N15-S12	-7.06	103.44	117.50
3	B	1	444	C16-N15-S12	-6.63	104.30	117.50
3	A	2	444	O14-S12-C01	-6.03	100.17	108.00
3	A	2	444	C24-C23-N15	-3.06	115.71	120.34
3	B	1	444	C24-C23-N15	-2.98	115.83	120.34
3	B	1	444	O42-C33-C26	-2.25	100.41	109.90
3	B	1	444	F20-C19-C16	-2.02	108.53	112.08
3	A	2	444	O14-S12-N15	2.41	109.89	106.78
3	A	2	444	C06-C01-S12	2.41	122.45	119.79
3	B	1	444	O14-S12-N15	2.41	109.90	106.78
3	B	1	444	C34-C33-C26	2.54	114.89	110.88
3	A	2	444	O13-S12-N15	3.15	110.84	106.78
3	B	1	444	C28-C23-N15	3.35	125.42	120.34
3	B	1	444	O13-S12-N15	3.69	111.55	106.78
3	A	2	444	C34-C33-C26	3.86	116.98	110.88
3	A	2	444	C28-C23-N15	3.89	126.25	120.34
3	A	2	444	C38-C33-C34	5.90	115.69	110.55
3	B	1	444	C38-C33-C34	6.68	116.38	110.55
3	A	2	444	C01-S12-N15	9.72	121.93	106.81
3	B	1	444	C01-S12-N15	9.92	122.24	106.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	444	3	0
3	B	1	444	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	279/293 (95%)	-0.01	16 (5%)	27 17	26, 46, 90, 113	0
1	B	279/293 (95%)	0.20	18 (6%)	22 13	26, 50, 96, 117	0
2	C	15/15 (100%)	1.48	6 (40%)	0 0	77, 85, 111, 111	0
2	D	15/15 (100%)	0.66	1 (6%)	21 12	54, 76, 114, 114	0
All	All	588/616 (95%)	0.15	41 (6%)	19 11	26, 50, 101, 117	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1311	THR	5.9
2	C	626	LEU	5.8
1	B	1310	ASP	4.5
1	B	1218	GLU	4.2
1	A	311	THR	4.1
1	B	1232	GLY	4.0
1	B	1315	PHE	3.9
1	B	1357	LEU	3.7
1	B	1318	LEU	3.6
1	A	316	GLN	3.6
1	B	1317	GLN	3.6
1	A	232	GLY	3.6
1	A	233	GLY	3.5
2	C	628	GLU	3.5
1	A	315	PHE	3.4
1	B	1194	GLU	3.4
1	B	1146	GLU	3.4
1	B	1195	GLU	3.3
1	B	1312	ALA	3.3
1	A	199	TRP	3.2
1	A	312	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	1628	GLU	3.0
1	A	234	LYS	2.9
1	B	1319	LEU	2.7
1	A	431	ILE	2.6
1	B	1231	SER	2.6
1	B	1316	GLN	2.6
1	A	192	SER	2.5
1	A	432	THR	2.5
1	B	1314	GLY	2.4
2	C	630	HIS	2.3
1	A	231	SER	2.3
1	A	270	GLU	2.2
1	A	313	GLY	2.2
2	C	627	THR	2.2
2	C	629	ARG	2.1
1	A	357	LEU	2.1
1	B	1284	SER	2.1
1	A	235	GLU	2.1
2	C	625	SER	2.1
1	B	1432	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	444	B	1	31/31	0.79	0.41	5.92	77,84,93,93	0
3	444	A	2	31/31	0.84	0.35	5.31	75,86,95,96	0

6.5 Other polymers

There are no such residues in this entry.