Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 04:42 PM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

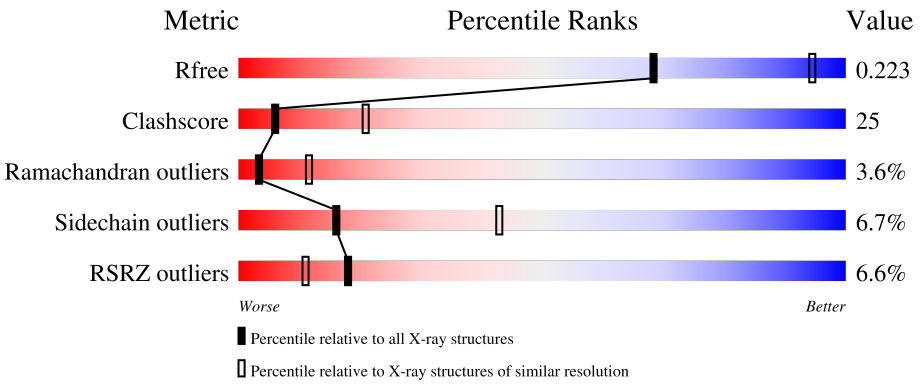
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5%, 54%, 35%, 6%, 5%
1	B	293	6%, 51%, 38%, 6%, • 5%
2	C	15	33%, 20%, 60%, 20%
2	D	15	7%, 47%, 40%, 13%

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	B	1	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	279	2265	1455	386	407	17	0	0	0
1	B	279	2265	1455	386	407	17	0	0	0

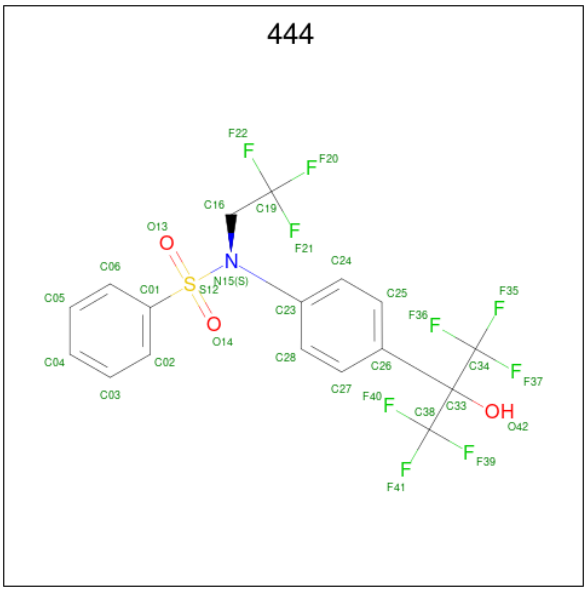
There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- 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: $C_{17}H_{12}F_9NO_3S$).



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

- Molecule 4 is water.

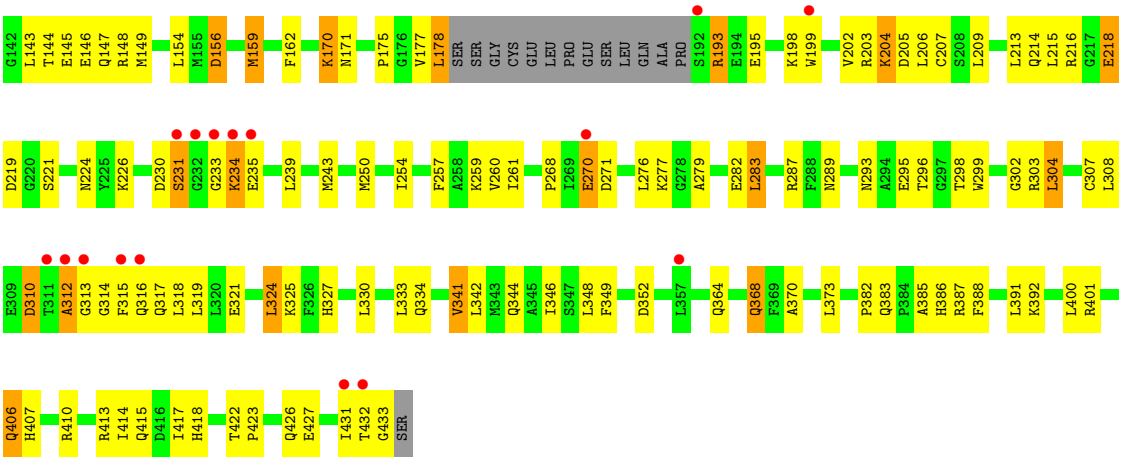
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	62	62	62	0	0
			Total	O		
4	B	66	66	66	0	0
			Total	O		
4	C	1	1	1	0	0
			Total	O		
4	D	6	6	6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

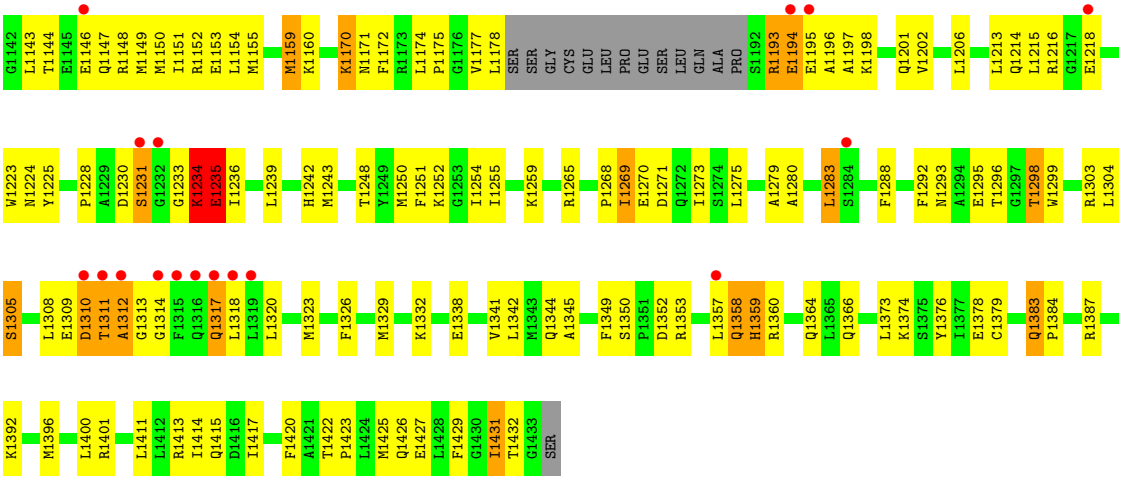
• Molecule 1: Orphan nuclear receptor PXR

Chain A:



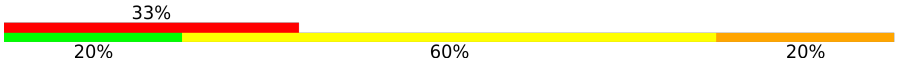
• Molecule 1: Orphan nuclear receptor PXR

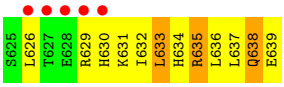
Chain B:



• Molecule 2: Nuclear Receptor Coactivator 1 isoform 3

Chain C:





- Molecule 2: Nuclear Receptor Coactivator 1 isoform 3

Chain D:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	4.96 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.240 0.220 , 0.223	Depositor DCC
R_{free} test set	1029 reflections (5.11%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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:HA	1:A:193:ARG:CZ	2.12	0.80
1:B:1254:ILE:HD12	1:B:1283:LEU:HB3	1.65	0.78
1:B:1383:GLN:CD	1:B:1383:GLN:H	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:144:THR:OG1	1:A:146:GLU:HG2	1.91	0.71
1:A:296:THR:O	1:A:298:THR:HG23	1.90	0.71
1:A:387:ARG:O	1:A:388:PHE:HB2	1.88	0.71
1:B:1431:ILE:H	1:B:1431:ILE:HD12	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:A:364:GLN:HE21	1:A:368:GLN:HE22	1.50	0.60
1:B:1213:LEU:HD23	1:B:1214:GLN:N	2.16	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:A:214:GLN:HG3	1:A:224:ASN:HD22	1.70	0.57
1:B:1415:GLN:HG2	1:B:1431:ILE:HG12	1.84	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:1170:LYS:HB2	4:B:3056:HOH:O	2.06	0.56
1:B:1273:ILE:HG23	2:D:1633:LEU:HD13	1.88	0.56
1:A:170:LYS:NZ	1:A:170:LYS:HB3	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:216:ARG:NH2	1:A:302:GLY:O	2.40	0.55
1:A:313:GLY:HA3	1:A:317:GLN:HB2	1.89	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:HH11	1:B:1265:ARG:HB3	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:A:277:LYS:HD3	2:C:630:HIS:CD2	2.46	0.50
1:B:1317:GLN:HA	1:B:1320:LEU:HD12	1.94	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:A:312:ALA:O	1:A:317:GLN:HG2	2.11	0.49
1:B:1213:LEU:HD21	1:B:1215:LEU:HD21	1.94	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:1153:GLU:HG2	4:B:3043:HOH:O	2.12	0.48
1:B:1175:PRO:HG2	1:B:1225:TYR:CE2	2.48	0.48
1:B:1201:GLN:CG	1:B:1413:ARG:HH11	2.26	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: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:1193:ARG:NH2	1:B:1197:ALA:H	2.10	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:A:145:GLU:O	1:A:149:MET:HE2	2.15	0.47
1:A:175:PRO:HD2	1:B:1223:TRP:CZ2	2.50	0.47
1:A:178:LEU:HD13	4:A:3042:HOH:O	2.13	0.47
1:B:1218:GLU:HA	1:B:1303:ARG:NH2	2.30	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
1:A:254:ILE:O	1:A:257:PHE:HB3	2.14	0.46
1:B:1265:ARG:NH1	1:B:1265:ARG:CB	2.78	0.46
2:C:637:LEU:C	2:C:638:GLN:HE21	2.18	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:1149:MET:HE3	1:B:1152:ARG:HD2	1.98	0.45
1:B:1283:LEU:HD13	1:B:1344:GLN:HB3	1.99	0.45
1:A:346:ILE:HD11	1:A:370:ALA:HA	1.99	0.45
1:B:1148:ARG:O	1:B:1152:ARG:HG3	2.17	0.45
1:B:1216:ARG:HH12	1:B:1305:SER:HB2	1.82	0.45
1:B:1251:PHE:O	1:B:1255:ILE:HG13	2.17	0.45
1:B:1270:GLU:OE2	2:D:1627:THR:HG21	2.17	0.45
1:A:205:ASP:O	1:A:410:ARG:NH1	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1193:ARG:HD3	1:B:1194:GLU:N	2.31	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:206:LEU:HD21	1:A:414:ILE:HD13	1.99	0.44
1:A:231:SER:HA	4:A:3113:HOH:O	2.17	0.44
1:A:259:LYS:HZ1	2:C:639:GLU:HG3	1.82	0.44
1:A:209:LEU:HD11	1:A:410:ARG:NH1	2.31	0.44
1:A:215:LEU:HD23	1:A:304:LEU:HB3	1.99	0.44
1:A:234:LYS:HE3	1:A:418:HIS:HD2	1.83	0.44
1:A:235:GLU:H	1:A:235:GLU:CD	2.20	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: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:1170:LYS:O	1:B:1171:ASN:HB2	2.17	0.44
1:B:1177:VAL:HG22	1:B:1178:LEU:HG	2.00	0.44
1:B:1193:ARG:O	1:B:1194:GLU:C	2.56	0.44
1:B:1293:ASN:OD1	1:B:1295:GLU:HB2	2.18	0.44
1:A:431:ILE:O	1:A:433:GLY:N	2.50	0.44
1:B:1265:ARG:HH11	1:B:1265:ARG:CB	2.30	0.44
2:D:1629:ARG:H	2:D:1629:ARG:HD3	1.83	0.44
1:A:303:ARG:HG2	1:A:303:ARG:HH11	1.82	0.44
1:B:1149:MET:HE3	1:B:1149:MET:HA	2.00	0.44
1:B:1193:ARG:HH21	1:B:1197:ALA:N	2.14	0.44
1:A:143:LEU:N	1:A:143:LEU:HD12	2.33	0.43
1:B:1239:LEU:O	1:B:1243:MET:HG2	2.18	0.43
2:C:626:LEU:O	2:C:630:HIS:ND1	2.51	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:1172:PHE:HE1	1:B:1174:LEU:HD21	1.84	0.43
1:B:1213:LEU:HD23	1:B:1213:LEU:C	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: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
2:C:629:ARG:HH11	2:C:629:ARG:HB3	1.84	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:A:257:PHE:O	1:A:261:ILE:HG13	2.20	0.42
1:A:312:ALA:C	1:A:314:GLY:H	2.22	0.42
1:B:1193:ARG:HH21	1:B:1197:ALA:H	1.68	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:A:234:LYS:HE3	1:A:418:HIS:CD2	2.55	0.42
1:A:321:GLU:HG3	1:A:324:LEU:H	1.85	0.42
1:B:1309:GLU:O	1:B:1311:THR:N	2.53	0.42
1:B:1312:ALA:C	1:B:1314:GLY:H	2.23	0.42
1:A:254:ILE:HD11	1:A:287:ARG:HD2	2.02	0.42
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.80	0.42
1:A:348:LEU:HD23	1:A:349:PHE:CE1	2.55	0.41
1:A:387:ARG:O	1:A:388:PHE:CB	2.61	0.41
1:B:1279:ALA:O	1:B:1280:ALA:C	2.57	0.41
1:B:1423:PRO:HB2	2:D:1632:ILE:CD1	2.50	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:1234:LYS:C	1:B:1236:ILE:H	2.23	0.41
1:B:1376:TYR:CD1	1:B:1376:TYR:C	2.93	0.41
1:B:1150:MET:O	1:B:1154:LEU:HD13	2.21	0.41
1:A:221:SER:HB2	1:B:1225:TYR:CE1	2.56	0.41
1:A:406:GLN:HE22	1:A:413:ARG:HH22	1.69	0.41
1:B:1143:LEU:HD13	1:B:1379:CYS:SG	2.61	0.41
1:B:1177:VAL:O	1:B:1178:LEU:HB2	2.21	0.41
1:B:1202:VAL:HG23	4:B:3044:HOH:O	2.21	0.41
1:B:1342:LEU:O	1:B:1345:ALA:HB3	2.21	0.41
2:C:635:ARG:C	2:C:635:ARG:HD3	2.41	0.41
1:B:1358:GLN:O	1:B:1360:ARG:N	2.54	0.41
1:A:318:LEU:O	1:A:321:GLU:HB3	2.21	0.40
1:A:319:LEU:HD22	1:A:325:LYS:HG3	2.04	0.40
1:A:352:ASP:OD2	1:A:401:ARG:CZ	2.70	0.40
1:A:383:GLN:O	1:A:386:HIS:N	2.45	0.40
1:A:177:VAL:HG11	1:B:1215:LEU:HD13	2.02	0.40
1:A:154:LEU:HD23	1:A:341:VAL:HG13	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:HB3	1:A:170:LYS:HZ3	1.86	0.40
1:A:226:LYS:HB2	1:A:226:LYS:HE3	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
1:B:1427:GLU:OE2	2:D:1632:ILE:HB	2.22	0.40
2:C:629:ARG:C	2:C:630:HIS:ND1	2.75	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%)	8 28
1	B	275/293 (94%)	244 (89%)	16 (6%)	15 (6%)	2 5
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%)	3 11

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 (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	248/260 (95%)	231 (93%)	17 (7%)	15 41
1	B	248/260 (95%)	235 (95%)	13 (5%)	23 55
2	C	15/15 (100%)	12 (80%)	3 (20%)	1 4
2	D	15/15 (100%)	13 (87%)	2 (13%)	4 12
All	All	526/550 (96%)	491 (93%)	35 (7%)	16 43

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

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

Mol	Chain	Res	Type
1	A	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 monosaccharides 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	-	31,32,32	6.17	20 (64%)	52,52,52	3.35	13 (25%)
3	444	B	1	-	31,32,32	6.28	20 (64%)	52,52,52	3.39	13 (25%)

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	-	-	11/45/45/45	0/2/2/2
3	444	B	1	-	-	11/45/45/45	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	444	O13-S12	15.51	1.60	1.43
3	B	1	444	O13-S12	15.48	1.60	1.43
3	A	2	444	O14-S12	14.86	1.60	1.43
3	B	1	444	O14-S12	14.77	1.59	1.43
3	B	1	444	C23-N15	14.29	1.64	1.44
3	A	2	444	C23-N15	13.83	1.64	1.44
3	B	1	444	C33-C26	9.04	1.66	1.53
3	B	1	444	C27-C26	8.41	1.52	1.39
3	A	2	444	C02-C01	8.25	1.51	1.38
3	B	1	444	C02-C01	8.23	1.51	1.38
3	A	2	444	C33-C26	8.22	1.65	1.53
3	B	1	444	C25-C26	8.20	1.52	1.39
3	A	2	444	C27-C26	8.05	1.52	1.39
3	A	2	444	C25-C26	7.84	1.51	1.39
3	B	1	444	C24-C23	7.77	1.54	1.39
3	A	2	444	C24-C23	7.56	1.54	1.39
3	A	2	444	C06-C01	7.12	1.50	1.38
3	B	1	444	C06-C01	6.93	1.49	1.38
3	A	2	444	C03-C02	5.02	1.49	1.38
3	B	1	444	C03-C02	5.00	1.49	1.38
3	B	1	444	C28-C23	4.55	1.48	1.39
3	A	2	444	C04-C03	4.53	1.50	1.38
3	A	2	444	C28-C23	4.47	1.48	1.39
3	B	1	444	C04-C03	4.37	1.49	1.38
3	B	1	444	C05-C04	4.36	1.49	1.38
3	A	2	444	C05-C04	4.27	1.49	1.38
3	A	2	444	C05-C06	4.13	1.47	1.38
3	B	1	444	C05-C06	4.06	1.47	1.38
3	B	1	444	C16-C19	3.85	1.55	1.50
3	A	2	444	C01-S12	3.73	1.81	1.76
3	B	1	444	C25-C24	3.29	1.44	1.38
3	B	1	444	C38-C33	3.12	1.60	1.54
3	B	1	444	C01-S12	2.89	1.80	1.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	444	C27-C28	2.79	1.43	1.38
3	A	2	444	C27-C28	2.77	1.43	1.38
3	A	2	444	S12-N15	-2.71	1.61	1.65
3	A	2	444	C16-C19	2.58	1.53	1.50
3	A	2	444	C38-C33	2.56	1.59	1.54
3	A	2	444	C25-C24	2.25	1.42	1.38
3	B	1	444	O42-C33	2.04	1.46	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1	444	C19-C16-N15	11.32	123.14	112.14
3	B	1	444	C01-S12-N15	11.23	122.24	106.92
3	A	2	444	C19-C16-N15	11.07	122.89	112.14
3	A	2	444	C01-S12-N15	11.00	121.93	106.92
3	A	2	444	C16-N15-S12	-9.73	103.44	117.00
3	A	2	444	O14-S12-O13	-9.47	104.17	119.52
3	B	1	444	O14-S12-O13	-9.24	104.55	119.52
3	B	1	444	C16-N15-S12	-9.11	104.30	117.00
3	B	1	444	O14-S12-C01	-7.84	98.13	108.05
3	A	2	444	O14-S12-C01	-6.22	100.17	108.05
3	B	1	444	C38-C33-C34	4.87	116.38	110.28
3	A	2	444	C38-C33-C34	4.32	115.69	110.28
3	B	1	444	O13-S12-N15	4.09	111.55	106.71
3	A	2	444	C28-C23-N15	4.08	126.25	120.16
3	A	2	444	C34-C33-C26	3.90	116.98	110.34
3	B	1	444	C28-C23-N15	3.52	125.42	120.16
3	A	2	444	O13-S12-N15	3.49	110.84	106.71
3	A	2	444	C24-C23-N15	-2.99	115.71	120.16
3	B	1	444	C24-C23-N15	-2.91	115.83	120.16
3	B	1	444	O14-S12-N15	2.70	109.90	106.71
3	A	2	444	O14-S12-N15	2.69	109.89	106.71
3	B	1	444	C34-C33-C26	2.68	114.89	110.34
3	A	2	444	C06-C01-S12	2.56	122.45	119.76
3	B	1	444	O42-C33-C26	-2.48	100.41	110.14
3	A	2	444	O42-C33-C26	-2.21	101.47	110.14
3	B	1	444	F20-C19-C16	-2.19	108.53	112.13

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	444	C19-C16-N15-S12
3	A	2	444	N15-C16-C19-F22
3	A	2	444	N15-C16-C19-F21
3	B	1	444	C19-C16-N15-S12
3	B	1	444	N15-C16-C19-F22
3	B	1	444	N15-C16-C19-F21
3	B	1	444	N15-C16-C19-F20
3	B	1	444	C28-C23-N15-C16
3	A	2	444	C28-C23-N15-C16
3	B	1	444	C24-C23-N15-C16
3	B	1	444	C06-C01-S12-O14
3	A	2	444	C06-C01-S12-O14
3	B	1	444	C02-C01-S12-O14
3	A	2	444	C02-C01-S12-O14
3	A	2	444	N15-C16-C19-F20
3	B	1	444	C06-C01-S12-N15
3	A	2	444	C16-N15-S12-O13
3	B	1	444	C02-C01-S12-N15
3	A	2	444	C24-C23-N15-C16
3	A	2	444	C06-C01-S12-N15
3	A	2	444	C02-C01-S12-N15
3	B	1	444	C16-N15-S12-O13

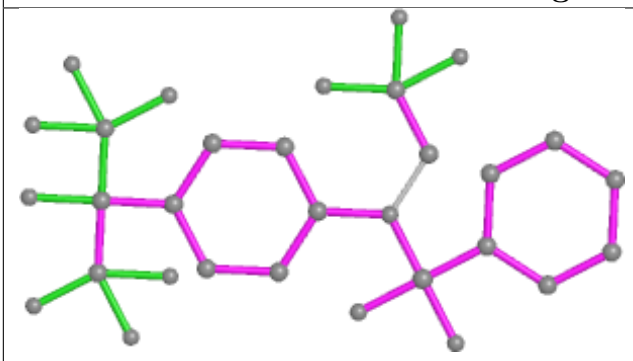
There are no ring outliers.

2 monomers are involved in 4 short contacts:

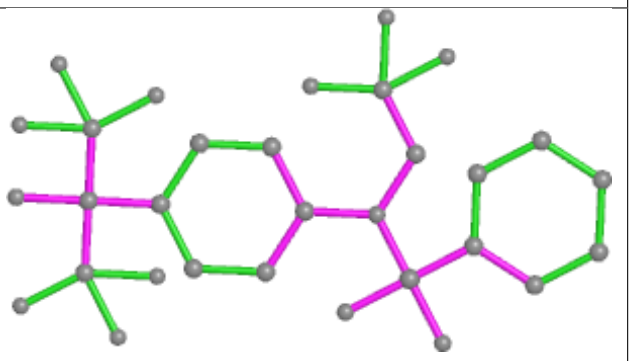
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	444	3	0
3	B	1	444	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

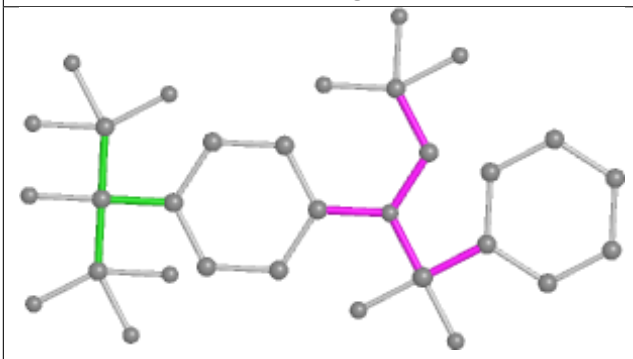
Ligand 444 A 2



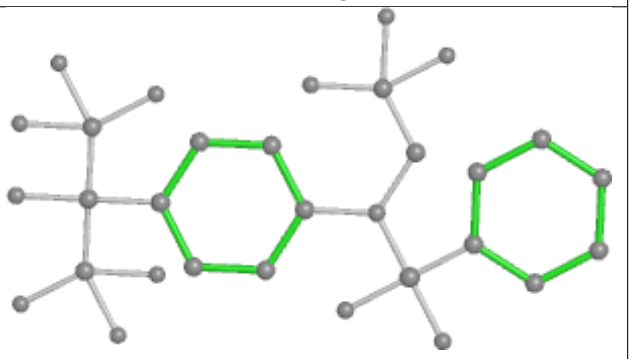
Bond lengths



Bond angles

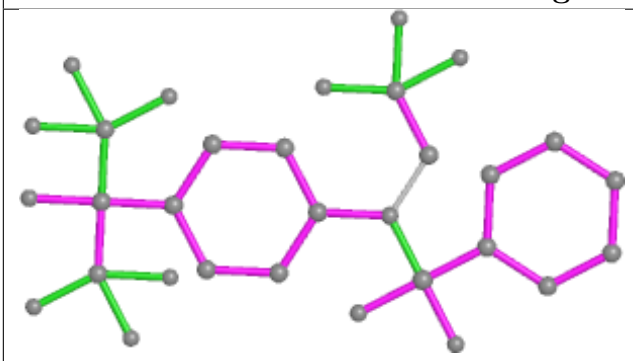


Torsions

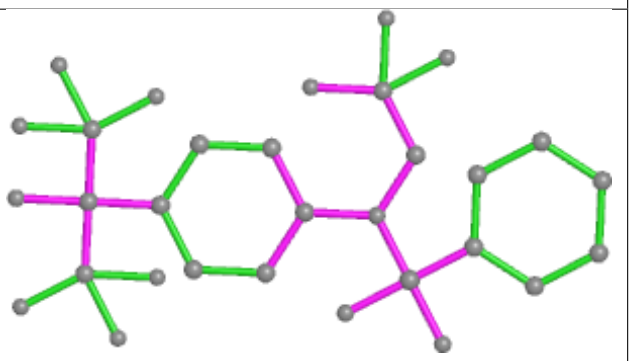


Rings

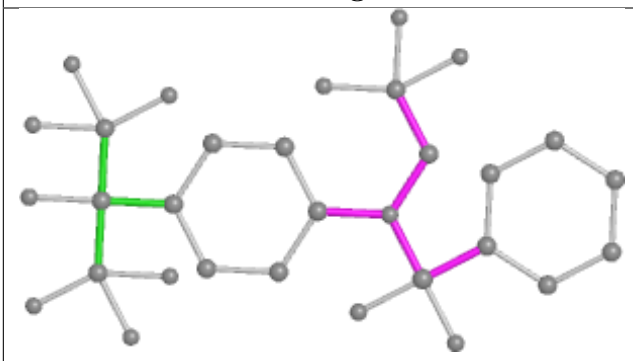
Ligand 444 B 1



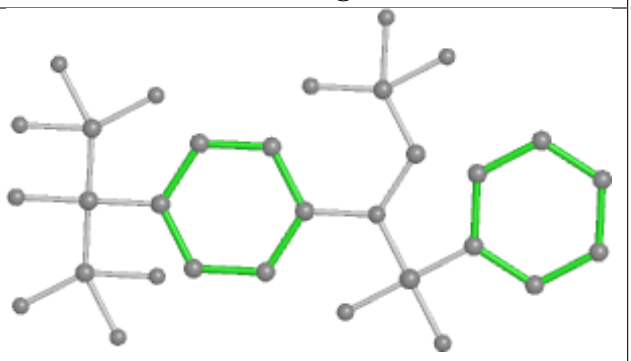
Bond lengths



Bond angles



Torsions



Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.02	16 (5%)	23	15	26, 46, 90, 113	0
1	B	279/293 (95%)	0.19	17 (6%)	21	13	26, 50, 96, 117	0
2	C	15/15 (100%)	1.46	5 (33%)	0	0	77, 85, 111, 111	0
2	D	15/15 (100%)	0.65	1 (6%)	17	10	54, 76, 114, 114	0
All	All	588/616 (95%)	0.13	39 (6%)	18	11	26, 50, 101, 117	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1311	THR	5.7
2	C	626	LEU	5.7
1	B	1310	ASP	4.3
1	B	1218	GLU	4.1
1	B	1232	GLY	4.0
1	A	311	THR	3.9
1	B	1315	PHE	3.8
1	B	1357	LEU	3.6
1	B	1318	LEU	3.6
1	A	232	GLY	3.5
1	A	233	GLY	3.5
1	A	316	GLN	3.5
1	B	1317	GLN	3.5
2	C	628	GLU	3.4
1	A	315	PHE	3.4
1	B	1194	GLU	3.3
1	B	1146	GLU	3.3
1	B	1312	ALA	3.3
1	B	1195	GLU	3.2
1	A	199	TRP	3.1
1	A	312	ALA	3.1

Continued on next page...

Continued from previous page...

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

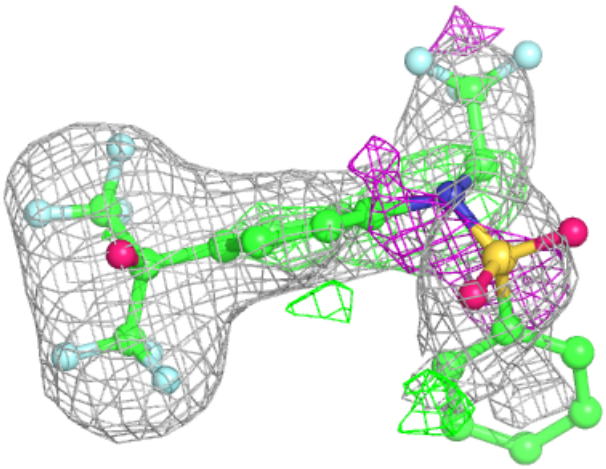
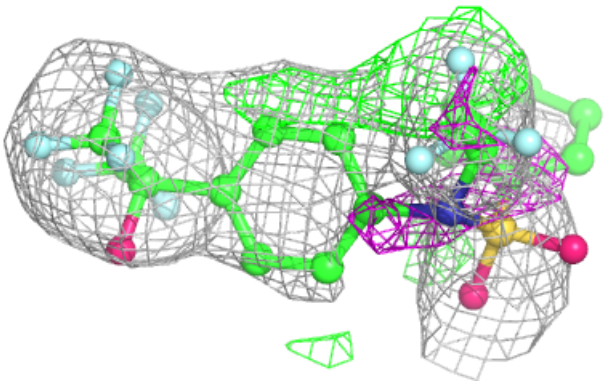
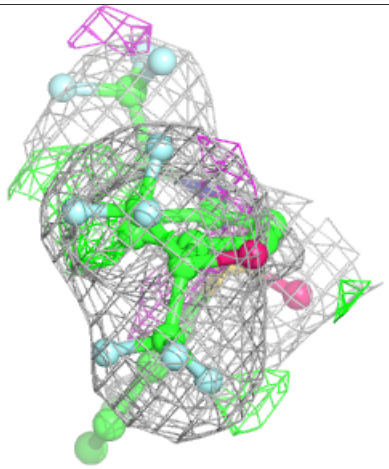
6.4 Ligands (i)

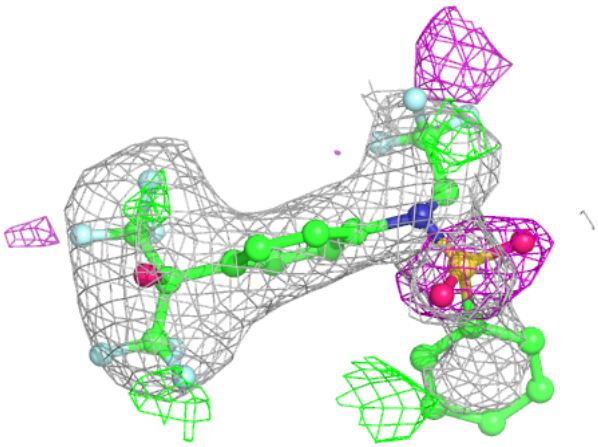
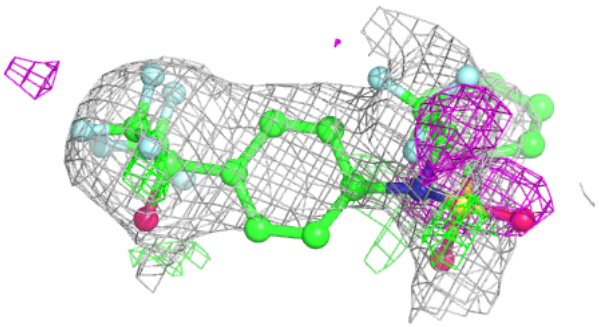
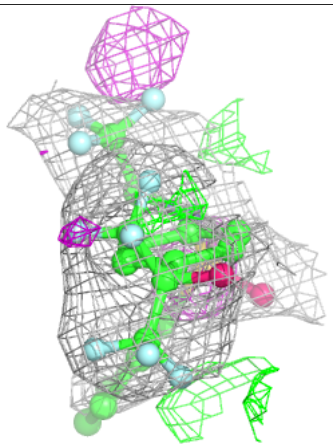
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 444 B 1: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around 444 A 2: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.