



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:29 AM GMT

PDB ID : 2HFP
Title : Crystal Structure of PPAR Gamma with N-sulfonyl-2-indole carboxamide ligands
Authors : Pokross, M.E.; Evdokimov, A.G.; Walter, R.L.; Mekel, M.J.; Hopkins, C.R.
Deposited on : 2006-06-25
Resolution : 2.00 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

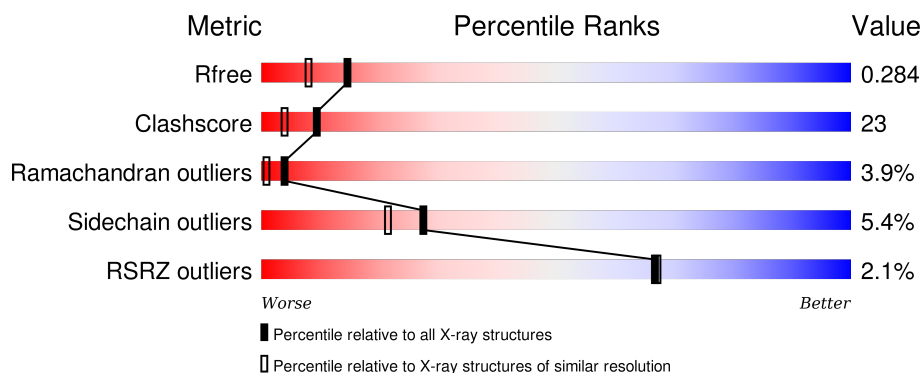
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	282	<div> <div></div> <div>68% 22% . . .</div> </div>
2	B	21	<div> <div>10%</div> <div>48% 10% 24% 19%</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	NSI	A	479	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2528 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 Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	2185	1411	356	408	10	0	0	0

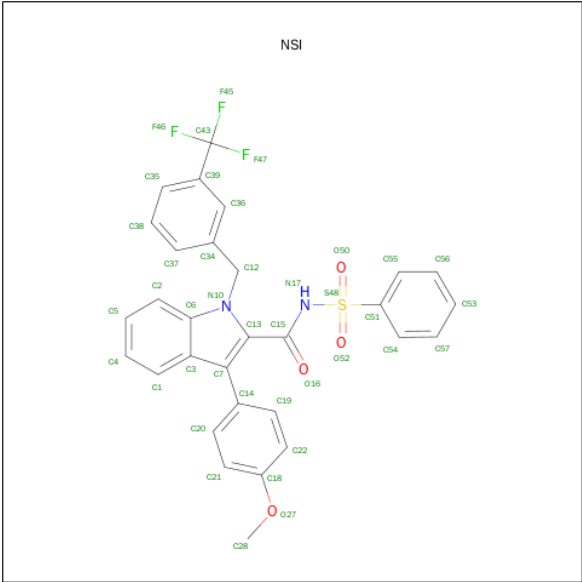
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	MET	-	CLONING ARTIFACT	UNP Q86U60
A	197	SER	-	CLONING ARTIFACT	UNP Q86U60
A	198	TYR	-	CLONING ARTIFACT	UNP Q86U60
A	199	TYR	-	CLONING ARTIFACT	UNP Q86U60
A	200	HIS	-	CLONING ARTIFACT	UNP Q86U60
A	201	HIS	-	CLONING ARTIFACT	UNP Q86U60
A	202	HIS	-	CLONING ARTIFACT	UNP Q86U60
A	203	HIS	-	CLONING ARTIFACT	UNP Q86U60
A	204	HIS	-	CLONING ARTIFACT	UNP Q86U60
A	205	HIS	-	CLONING ARTIFACT	UNP Q86U60

- Molecule 2 is a protein called SRC Peptide Fragment.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	17	141	86	29	26	0	0	0

- Molecule 3 is 3-(4-METHOXYPHENYL)-N-(PHENYLSULFONYL)-1-[3-(TRIFLUOROMETHYL)BENZYL]-1H-INDOLE-2-CARBOXAMIDE (three-letter code: NSI) (formula: C₃₀H₂₃F₃N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 40	C 30	F 3	N 2	O 4	S 1	0	0
3	A	1	Total 40	C 30	F 3	N 2	O 4	S 1	0	0

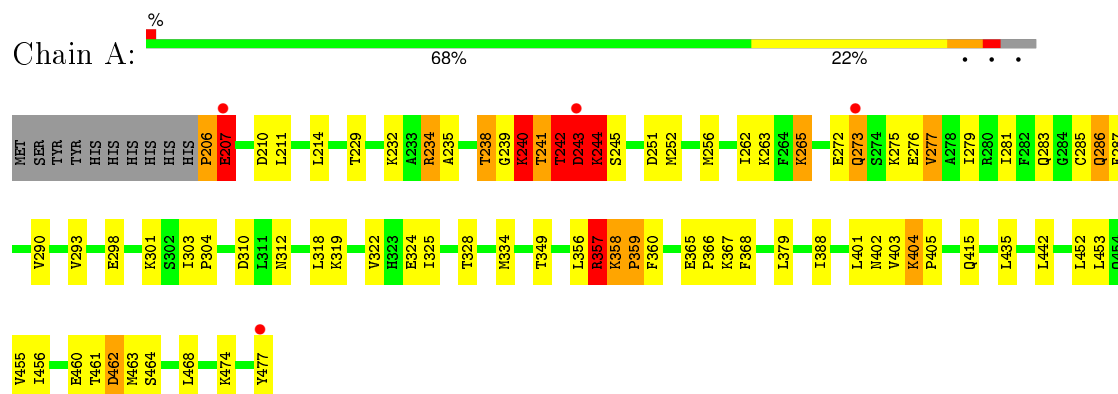
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	5	Total	O	0	0
			5	5		

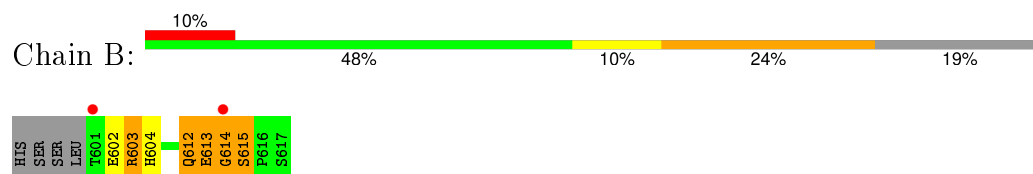
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: Peroxisome proliferator-activated receptor gamma



- Molecule 2: SRC Peptide Fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.49 Å 77.18 Å 82.08 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.80 – 2.00 39.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.80-2.00) 93.5 (39.82-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.285 0.202 , 0.284	Depositor DCC
R_{free} test set	1003 reflections (5.46%)	DCC
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.0	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	0 of 19405 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2528	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.79	2/2224 (0.1%)	0.85	2/2996 (0.1%)
2	B	0.57	0/143	0.94	0/189
All	All	0.78	2/2367 (0.1%)	0.86	2/3185 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	CYS	CB-SG	-5.57	1.72	1.81
1	A	349	THR	C-N	-5.50	1.21	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	251	ASP	CB-CG-OD1	5.34	123.11	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	PRO	Peptide
1	A	240	LYS	Peptide
1	A	242	THR	Peptide
1	A	243	ASP	Peptide
1	A	244	LYS	Peptide
1	A	357	ARG	Peptide
2	B	613	GLU	Peptide
2	B	614	GLY	Peptide

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	2185	0	2249	98	1
2	B	141	0	143	12	0
3	A	80	0	46	6	0
4	A	117	0	0	9	1
4	B	5	0	0	1	0
All	All	2528	0	2438	110	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 23.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:612:GLN:HE21	2:B:612:GLN:CA	1.54	1.19
2:B:612:GLN:NE2	2:B:612:GLN:HA	1.50	1.13
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.28	1.10
1:A:334:MET:CE	1:A:368:PHE:CD1	2.41	1.03
1:A:461:THR:O	1:A:462:ASP:HB2	1.65	0.96
1:A:404:LYS:HD2	4:A:127:HOH:O	1.70	0.92
2:B:602:GLU:HB2	2:B:604:HIS:H	1.37	0.90
1:A:334:MET:HE3	1:A:368:PHE:CE1	2.08	0.89
1:A:402:ASN:ND2	4:A:111:HOH:O	1.95	0.88
1:A:452:LEU:O	1:A:456:ILE:HD13	1.73	0.88
1:A:334:MET:HE3	1:A:368:PHE:CD1	2.09	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLN:NE2	4:A:70:HOH:O	2.06	0.87
2:B:602:GLU:HB3	2:B:603:ARG:HB3	1.60	0.83
1:A:334:MET:HE1	1:A:368:PHE:CD1	2.12	0.82
1:A:242:THR:O	1:A:244:LYS:HB3	1.79	0.82
1:A:360:PHE:HZ	1:A:463:MET:CE	1.94	0.81
1:A:360:PHE:CZ	1:A:463:MET:CE	2.66	0.79
1:A:367:LYS:HZ1	3:A:479:NSI:HN17	1.29	0.78
2:B:612:GLN:HE21	2:B:612:GLN:HA	0.66	0.76
1:A:402:ASN:HA	4:A:111:HOH:O	1.86	0.75
2:B:612:GLN:NE2	2:B:612:GLN:CA	2.28	0.73
1:A:334:MET:HE1	1:A:368:PHE:CG	2.25	0.72
2:B:602:GLU:HB2	2:B:604:HIS:N	2.04	0.72
1:A:276:GLU:OE2	1:A:357:ARG:HD3	1.91	0.71
1:A:360:PHE:CZ	1:A:463:MET:HE1	2.25	0.71
1:A:452:LEU:O	1:A:456:ILE:CD1	2.40	0.70
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.74	0.68
1:A:239:GLY:O	1:A:240:LYS:CB	2.42	0.68
1:A:252:MET:O	1:A:256:MET:HG3	1.95	0.65
2:B:602:GLU:HB3	2:B:603:ARG:CB	2.26	0.65
1:A:357:ARG:NH2	1:A:460:GLU:OE2	2.28	0.65
1:A:275:LYS:NZ	4:A:39:HOH:O	1.82	0.65
1:A:357:ARG:HG2	4:A:40:HOH:O	1.98	0.64
1:A:367:LYS:NZ	3:A:479:NSI:HN17	1.94	0.64
1:A:334:MET:CE	1:A:368:PHE:HA	2.28	0.64
1:A:206:PRO:CB	1:A:207:GLU:CG	2.75	0.64
1:A:238:THR:CG2	1:A:240:LYS:HD3	2.27	0.64
1:A:452:LEU:HG	1:A:456:ILE:HD11	1.79	0.63
1:A:357:ARG:HH22	1:A:460:GLU:CD	2.01	0.63
1:A:239:GLY:O	1:A:240:LYS:CG	2.47	0.63
1:A:286:GLN:NE2	1:A:464:SER:O	2.33	0.61
1:A:234:ARG:O	1:A:238:THR:HB	2.01	0.61
1:A:324:GLU:O	1:A:328:THR:HG23	2.01	0.61
2:B:602:GLU:HB3	2:B:603:ARG:CA	2.31	0.60
1:A:404:LYS:N	1:A:405:PRO:HD2	2.17	0.59
1:A:239:GLY:O	1:A:240:LYS:HB2	2.02	0.59
1:A:283:GLN:HE22	1:A:464:SER:H	1.51	0.59
1:A:452:LEU:HG	1:A:456:ILE:CD1	2.33	0.59
1:A:241:THR:OG1	1:A:242:THR:N	2.36	0.58
1:A:206:PRO:HB3	1:A:207:GLU:HG2	1.83	0.58
1:A:206:PRO:HG2	1:A:211:LEU:HD21	1.85	0.58
1:A:239:GLY:O	1:A:240:LYS:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ILE:O	1:A:265:LYS:HB2	2.04	0.58
1:A:310:ASP:OD2	1:A:312:ASN:HB2	2.04	0.58
1:A:334:MET:HE1	1:A:368:PHE:HA	1.86	0.56
1:A:206:PRO:HA	1:A:207:GLU:HB3	1.87	0.56
1:A:402:ASN:CA	4:A:111:HOH:O	2.49	0.56
1:A:252:MET:CE	1:A:277:VAL:HG11	2.36	0.55
1:A:206:PRO:HD2	1:A:415:GLN:OE1	2.07	0.55
1:A:358:LYS:CB	1:A:359:PRO:HD3	2.36	0.55
2:B:602:GLU:CB	2:B:603:ARG:CA	2.84	0.55
1:A:334:MET:CE	1:A:368:PHE:CE1	2.80	0.55
1:A:239:GLY:O	1:A:240:LYS:CD	2.56	0.53
3:A:478:NSI:H122	3:A:478:NSI:O16	2.07	0.53
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.38	0.53
1:A:206:PRO:HB2	1:A:207:GLU:HG3	1.90	0.53
1:A:325:ILE:HD12	1:A:388:ILE:HG23	1.91	0.53
1:A:206:PRO:CB	1:A:207:GLU:HG2	2.39	0.52
1:A:460:GLU:O	1:A:463:MET:HB2	2.09	0.52
1:A:206:PRO:CB	1:A:207:GLU:HG3	2.39	0.52
1:A:286:GLN:HG3	1:A:287:PHE:N	2.22	0.51
1:A:334:MET:HE2	1:A:368:PHE:HA	1.93	0.51
2:B:614:GLY:O	2:B:615:SER:OG	2.28	0.51
1:A:272:GLU:HB3	1:A:275:LYS:HD2	1.92	0.51
1:A:206:PRO:HB3	1:A:207:GLU:CG	2.40	0.51
1:A:207:GLU:O	1:A:207:GLU:HG3	2.12	0.50
1:A:235:ALA:HB1	1:A:241:THR:HG22	1.93	0.49
1:A:241:THR:OG1	1:A:243:ASP:HB3	2.12	0.49
1:A:360:PHE:CD1	3:A:479:NSI:H282	2.47	0.49
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.59	0.49
1:A:379:LEU:HD11	1:A:435:LEU:HD21	1.94	0.48
1:A:404:LYS:N	1:A:405:PRO:CD	2.77	0.48
1:A:455:VAL:HG13	1:A:456:ILE:HD12	1.94	0.48
1:A:281:ILE:HD13	1:A:356:LEU:HD11	1.96	0.47
1:A:301:LYS:HD2	4:B:57:HOH:O	2.15	0.47
1:A:229:THR:OG1	1:A:232:LYS:HD2	2.15	0.46
1:A:206:PRO:CA	1:A:207:GLU:HB3	2.46	0.46
1:A:303:ILE:O	1:A:304:PRO:C	2.53	0.46
1:A:318:LEU:O	1:A:319:LYS:C	2.54	0.46
1:A:252:MET:HE3	1:A:277:VAL:HG11	1.98	0.45
1:A:360:PHE:CZ	1:A:463:MET:HE2	2.47	0.45
1:A:461:THR:O	1:A:462:ASP:CB	2.45	0.45
1:A:474:LYS:HZ2	2:B:603:ARG:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:N	1:A:456:ILE:HD12	2.33	0.44
1:A:358:LYS:CB	1:A:359:PRO:CD	2.95	0.44
1:A:453:LEU:HD13	3:A:479:NSI:H57	2.01	0.43
1:A:206:PRO:CA	1:A:207:GLU:CB	2.97	0.43
1:A:298:GLU:OE2	4:A:122:HOH:O	2.22	0.42
1:A:365:GLU:N	1:A:366:PRO:CD	2.82	0.42
1:A:360:PHE:CE1	1:A:463:MET:CE	3.03	0.42
1:A:238:THR:HG23	1:A:239:GLY:O	2.19	0.41
1:A:263:LYS:C	1:A:265:LYS:H	2.24	0.41
1:A:328:THR:HG22	1:A:442:LEU:HD11	2.02	0.41
1:A:360:PHE:CE1	1:A:463:MET:HE2	2.55	0.41
1:A:279:ILE:O	1:A:283:GLN:HG2	2.21	0.41
1:A:207:GLU:OE2	1:A:210:ASP:OD2	2.39	0.41
1:A:404:LYS:CD	4:A:127:HOH:O	2.47	0.41
1:A:290:VAL:HG13	1:A:468:LEU:HD23	2.03	0.41
1:A:272:GLU:HG2	1:A:275:LYS:HD2	2.03	0.40
1:A:281:ILE:HA	3:A:478:NSI:H21	2.04	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:477:TYR:CE1	4:A:21:HOH:O[4_555]	1.80	0.40

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	270/282 (96%)	249 (92%)	12 (4%)	9 (3%)	5	1
2	B	15/21 (71%)	9 (60%)	4 (27%)	2 (13%)	0	0
All	All	285/303 (94%)	258 (90%)	16 (6%)	11 (4%)	4	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	240	LYS
1	A	241	THR
1	A	245	SER
1	A	358	LYS
2	B	615	SER
1	A	243	ASP
1	A	273	GLN
2	B	603	ARG
1	A	359	PRO
1	A	462	ASP

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	245/255 (96%)	233 (95%)	12 (5%)	31	25
2	B	16/20 (80%)	14 (88%)	2 (12%)	6	3
All	All	261/275 (95%)	247 (95%)	14 (5%)	27	21

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	214	LEU
1	A	238	THR
1	A	242	THR
1	A	244	LYS
1	A	265	LYS
1	A	277	VAL
1	A	286	GLN
1	A	357	ARG
1	A	401	LEU
1	A	403	VAL
1	A	404	LYS

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Mol	Chain	Res	Type
2	B	612	GLN
2	B	613	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	312	ASN
1	A	345	GLN
1	A	412	ASN
1	A	444	GLN
1	A	470	GLN
2	B	612	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	NSI	A	478	-	40,44,44	2.35	6 (15%)	54,65,65	1.91	11 (20%)
3	NSI	A	479	-	40,44,44	2.19	4 (10%)	54,65,65	2.79	10 (18%)

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	NSI	A	478	-	-	0/27/31/31	0/5/5/5
3	NSI	A	479	-	-	0/27/31/31	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	479	NSI	C51-S48	-9.39	1.62	1.76
3	A	478	NSI	C51-S48	-9.05	1.63	1.76
3	A	479	NSI	C7-C14	-7.67	1.40	1.49
3	A	478	NSI	C15-N17	-6.66	1.32	1.39
3	A	478	NSI	C7-C14	-5.76	1.43	1.49
3	A	478	NSI	S48-N17	-4.94	1.54	1.64
3	A	479	NSI	S48-N17	-4.52	1.55	1.64
3	A	479	NSI	C15-N17	-2.32	1.36	1.39
3	A	478	NSI	C22-C19	2.08	1.42	1.38
3	A	478	NSI	C4-C1	2.18	1.41	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	479	NSI	O50-S48-O52	-15.33	99.20	119.54
3	A	478	NSI	O50-S48-O52	-8.95	107.67	119.54
3	A	479	NSI	C1-C3-C7	-4.47	130.62	136.11
3	A	478	NSI	C1-C3-C7	-4.15	131.01	136.11
3	A	478	NSI	C51-S48-N17	-3.08	101.94	105.93
3	A	479	NSI	O52-S48-C51	-2.31	105.03	107.96
3	A	479	NSI	C12-C34-C36	-2.18	116.74	120.30
3	A	478	NSI	C12-C34-C36	-2.10	116.87	120.30
3	A	478	NSI	O52-S48-C51	-2.03	105.39	107.96
3	A	479	NSI	C28-O27-C18	2.02	122.24	117.51
3	A	478	NSI	O50-S48-N17	2.45	113.88	106.79
3	A	479	NSI	C35-C39-C43	2.56	123.83	119.99
3	A	478	NSI	C19-C14-C7	2.65	124.90	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	479	NSI	O50-S48-N17	2.66	114.49	106.79
3	A	478	NSI	C7-C13-N10	2.66	110.86	108.24
3	A	479	NSI	C56-C55-C51	2.87	122.06	118.95
3	A	478	NSI	O52-S48-N17	2.94	115.32	106.79
3	A	478	NSI	C57-C54-C51	3.12	122.33	118.95
3	A	478	NSI	O50-S48-C51	3.44	112.32	107.96
3	A	479	NSI	C51-S48-N17	4.21	111.39	105.93
3	A	479	NSI	O50-S48-C51	8.42	118.61	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	478	NSI	2	0
3	A	479	NSI	4	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 [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	272/282 (96%)	0.08	4 (1%) 76 77	16, 28, 52, 73	0
2	B	17/21 (80%)	0.39	2 (11%) 6 6	24, 35, 60, 63	0
All	All	289/303 (95%)	0.09	6 (2%) 67 67	16, 28, 55, 73	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	TYR	5.2
1	A	243	ASP	4.2
1	A	207	GLU	3.3
2	B	614	GLY	3.2
2	B	601	THR	2.7
1	A	273	GLN	2.6

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(\AA^2)	Q<0.9
3	NSI	A	479	40/40	0.84	0.17	2.06	32,46,59,61	0
3	NSI	A	478	40/40	0.97	0.12	-0.13	13,25,39,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.